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Search for heavy Higgs bosons from a g2HDM in multilepton plus b**-jets final states in** p p **collisions at 13 TeV with the ATLAS detector**

The ATLAS Collaboration

A search for new heavy scalars with flavour-violating decays in final states with multiple leptons and *b*-tagged jets is presented. The results are interpreted in terms of a general two-Higgs-doublet-model involving an additional scalar with couplings to the top-quark and the three up-type quarks (ρ_{tt} , ρ_{tc} , and ρ_{tu}). The targeted signals lead to final states with either a same-sign top-quark pair, three top-quarks, or four top-quarks. The search is based on a dataset s and same-sign top-quark pair, three top-quarks, or four top-quarks. The search is based on a dataset of proton-proton collisions at $\sqrt{s} = 13$ TeV recorded with the ATLAS detector during Run 2 of the Large Hadron Collider, corresponding to an integrated luminosity of 139 fb−¹ . Events are categorised depending on the multiplicity of light charged leptons (electrons or muons), total lepton charge, and a deep-neural-network-based categorisation to enhance the purity of each of the signals. A mild excess is observed over the Standard Model expectation corresponding to a local significance of 2.81 standard deviations for a signal with $m_H = 1000$ GeV and $\rho_{tt} = 0.32$, $\rho_{tc} = 0.05$, and $\rho_{tu} = 0.85$. Exclusion limits at 95% confidence are set on the mass and couplings of the heavy Higgs boson. Masses of an additional scalar boson m_H between 200-630 (200-840) GeV with couplings $\rho_{tt} = 0.4$, $\rho_{tc} = 0.2$, and $\rho_{tu} = 0.2$ are observed (expected) to be excluded at 95% confidence level. Additional interpretations are provided in models of *R*-parity violating supersymmetry, motivated by the recent flavour and $(g - 2)$ _µ anomalies.

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1 Introduction

Several extensions of the Standard Model propose the augmentation of the Higgs sector by the addition of a second complex Higgs doublet [\[1,](#page-34-0) [2\]](#page-34-1) (2HDM), giving rise to five Higgs bosons: two CP-even scalar fields *h* and *H*, one CP-odd pseudo-scalar *A*, and two charged fields *H* ± . The two CP-even scalars are expected to mix, however, the measurement of Higgs boson properties has revealed no deviations from the expectations of the Standard Model. This would mean that extra scalars from 2HDMs have to be either very heavy (decoupling limit) or have a vanishingly small mixing with the SM Higgs (alignment limit). In order to avoid flavour changing neutral Higgs (FCNH) couplings mediated by the SM Higgs, a discrete Z_2 symmetry is usually imposed. Searches for heavy scalars or pseudo-scalars with flavour-conserving decays have been performed extensively in ATLAS [\[3–](#page-34-2)[10\]](#page-34-3) and CMS [\[11](#page-34-4)[–23\]](#page-35-0). However, if the Z_2 symmetry is dropped, alignment automatically emerges when all heavy Higgs quartic couplings are $O(1)$ [\[24\]](#page-35-1). Therefore, models without Z_2 symmetry can lead naturally to the alignment limit and predict FCNH couplings in the heavy Higgs sector, while respecting the SM-like nature of the *h*(125) discovered at the LHC.

The search presented in this paper targets such a general two Higgs doublet model (g2HDM) without *Z*² symmetry, where the heavy Higgs bosons feature FCNH couplings. Only couplings involving top-quarks are considered: ρ_{tt} , ρ_{tc} , and ρ_{tu} . The ρ_{AB} parameters indicate the coupling of the heavy Higgs boson to particles *A* and *B*. The notation ρ_{tq} is used to refer to both the ρ_{tc} and ρ_{tu} couplings. These kinds of g2HDMs with extra top Yukawa couplings are phenomenologically interesting since they can explain the generation of the baryon asymmetry through the couplings ρ_{tt} or ρ_{tc} [\[25\]](#page-35-2). No distinction is performed between the different chiralities in the coupling, and an effective coupling $\rho_{tq} = \sqrt{\hat{\rho}_t^2}$ $t_{L}q_{R} + \hat{\rho}_{q}^{2}$ $q_{L}t_{R}$ / $\frac{1}{\sqrt{2}}$ is used, where the hat symbol is used to denote the original couplings in the g2HDM lagrangian.

The production and decay modes at tree level considered in the analysis are shown in Figure [1.](#page-2-0) The presence of the ρ_{ta} coupling opens the possibility of same-sign top production, as shown in Figures [1\(a\)](#page-2-1) (sstt) and $1(b)$ (ttq), and also three-top production, as shown in Figures $1(c)$ (ttt) and $1(d)$ (tttq). The three-top signature has been highlighted as a sensitive probe of new physics [\[26–](#page-35-3)[29\]](#page-36-0). Additionally, four-top quarks can be produced, as shown in Figure $1(e)$ (tttt). The targeted final state is characterised by multiple leptons (electrons and muons) and multiple jets containing *b*-flavoured hadrons (*b*-jets). Many of the production modes are expected to be charge-asymmetric (with preference to positively charged), and this feature is exploited in the search. The relevance of each production mode depends on the chosen coupling. A benchmark of $\rho_{tt} = 0.4$ and $\rho_{tq} = 0.2$ is chosen to guide the analysis design and optimisation. The values are chosen so that the signal would be responsible for the higher $t\bar{t}W$ and $t\bar{t}t\bar{t}$ yields observed in ATLAS analyses [\[30](#page-36-1)[–34\]](#page-36-2). For the chosen couplings, the *tH* production cross section is two orders of magnitude larger than *ttH* production, and three orders of magnitude larger than same-sign tops production via *t*-channel *H*.

This analysis is the first to target BSM production leading to three-top final states and the first to probe the g2HDM. The production of four-tops in the SM or via heavy scalars has been explored previously by ATLAS [\[33](#page-36-3)[–37\]](#page-36-4) and CMS [\[38–](#page-36-5)[41\]](#page-36-6). Limits on the couplings can be derived from LHC Higgs measurements, *B* physics, and assuming perturbativity [\[42\]](#page-36-7), leading to $\rho_{tt} < 2$, $\hat{\rho}_{tc} < 1.5$, and $\hat{\rho}_{ct} < 0.1$, or equivalently ρ_{tc} < 1.06. In addition, $K - \bar{K}$ mixing provides the constraint $\hat{\rho}_{ct}$ < 0.14 [\[43\]](#page-37-0), and $D - \bar{D}$ mixing provides the constraint $|\hat{\rho}_{tc}\hat{\rho}_{tu}^*| < 0.02$ [\[43\]](#page-37-0), which translates to $|\rho_{tc}\hat{\rho}_{tu}^*| < 0.01$ assuming a negligible $\hat{\rho}_{ut}$. These constraints are derived assuming $m_H \approx m_{H^+} = 500$ GeV, and become weaker for higher masses.

Two additional signal models based on R-parity-violating supersymmetry (RPV SUSY) are used to interpret the results of the search. The models are motivated by the recent flavour anomalies [\[44](#page-37-1)[–51\]](#page-37-2) and $(g - 2)_{\mu}$

Figure 1: Signal diagrams for the dominant production and decay modes of the heavy scalar considered in the analysis. The subsequent decay can lead to a final state with high multiplicity of leptons and *b*-jets which is targeted by the search. Single production through gluon fusion is not considered since the decay does not lead to the relevant final state.

Figure 2: Signal diagrams for the RPV SUSY signals used as additional interpretation in the analysis. The subsequent decay can lead to a final state with high multiplicity of leptons and *b*-jets which is targeted by the search.

anomaly [\[52\]](#page-37-3), and can provide a successful explanation with different choices of particles, masses, and couplings [\[53–](#page-37-4)[62\]](#page-38-0). The first model features electroweakino production (wino or Higgsino) which decays via a lepton-number-violating RPV coupling of the $LQ\bar{D}$ type to a lepton and third-generation quarks. The corresponding term in the superpotential has the form $\lambda'_{133}L_iQ_3\bar{D}_3$, where *i* ∈ 2, 3 is a generation index, and L, Q, \bar{D} are the lepton doublet, quark doublet, and down-type quark singlet superfields, respectively. Relevant diagrams for the production and decay are shown in Figures $2(a)$ and $2(b)$. The second model features direct smuon production decaying to a bino-like neutralino, which in turn decays via the same RPV coupling (λ'_{i33}) , as shown in Figure [2\(c\).](#page-2-8)

2 ATLAS detector

The ATLAS experiment [\[63\]](#page-38-1) at the LHC is a multipurpose particle detector with a forward–backward symmetric cylindrical geometry and nearly 4π coverage in solid angle.^{[1](#page-3-0)} It consists of an inner tracking
detector (ID) surrounded by a thin superconducting solenoid providing a 2.7 axial magnetic field detector (ID) surrounded by a thin superconducting solenoid providing a 2T axial magnetic field, electromagnetic (EM) and hadron calorimeters, and a muon spectrometer (MS). The inner tracking detector covers the pseudorapidity range $|\eta| < 2.5$. It consists of silicon pixel, silicon microstrip and transition radiation tracking detectors; the innermost layer is 33 mm from the beamline [\[64,](#page-38-2) [65\]](#page-38-3). Lead/liquid-argon (LAr) sampling calorimeters provide electromagnetic energy measurements with high granularity. A steel/scintillator-tile hadron calorimeter covers the central pseudorapidity range ($|\eta| < 1.7$). The endcap and forward regions are instrumented with LAr calorimeters for both the EM and hadronic energy measurements up to $|\eta| = 4.9$. The muon spectrometer surrounds the calorimeters and is based on three large superconducting air-core toroidal magnets with eight coils each. The field integral of the toroids ranges between 2.0 and 6.0 T·m across most of the detector. The muon spectrometer includes a system of precision tracking chambers and fast detectors for triggering. A two-level trigger system is used to select events [\[66\]](#page-38-4). The first-level trigger is implemented in hardware and uses a subset of the detector information to keep the accepted rate below approximately 100 kHz. This is followed by a software-based trigger that reduces the accepted event rate to approximately 1 kHz on average depending on the data-taking conditions. An extensive software suite [\[67\]](#page-38-5) is used for real and simulated data reconstruction and analysis, for operation and in the trigger and data acquisition systems of the experiment.

3 Data and simulated event samples

A dataset of *pp* collisions at \sqrt{s} = 13 TeV collected by the ATLAS experiment during 2015–2018 and corresponding to an integrated luminosity of 139 fb−¹ is used. The number of additional *pp* interactions per bunch crossing (pile-up) in this dataset ranges from about 8 to 70, with an average of 34. Only events recorded under stable beam conditions and for which all detector subsystems were known to be in a good operating condition are used. The trigger requirements are discussed in Section [5.](#page-9-0)

Monte Carlo (MC) simulation samples were produced for the different signal and background processes. Table [1](#page-6-0) shows the configurations used in this analysis, with the samples in parentheses and in grey indicating those used to estimate the systematic uncertainties. All simulated samples, except those produced with the SHERPA [\[68\]](#page-38-6) event generator, utilised EvrGen 1.2.0 [\[69\]](#page-38-7) to model the decays of heavy-flavour hadrons. All samples showered with PYTHIA use the A14 tune [\[70\]](#page-38-8), whereas those showered with HERWIG use the H7-UE set of tuned parameters [\[71\]](#page-38-9). Pile-up was modelled using events from minimum-bias interactions generated with Pythia 8.186 [\[72\]](#page-38-10) with the A3 set of tuned parameters [\[73\]](#page-38-11) (referred to as the 'tune'), and overlaid onto the simulated hard-scatter events according to the luminosity profile of the recorded data. The generated events were processed through either a full simulation of the ATLAS detector geometry and response using Geant4 [\[74\]](#page-38-12), or a faster simulation where the full Geant4 simulation of the calorimeter response is replaced by a detailed parameterisation of the shower shapes [\[75\]](#page-39-0). In both cases, the simulated events were processed through the same reconstruction software as the dataset of *pp* collisions. Corrections

¹ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the *z*-axis along the beam pipe. The *x*-axis points from the IP to the centre of the LHC ring, and the y-axis points upwards. Cylindrical coordinates (*r*, φ) are used in the transverse plane, φ being the azimuthal angle around the *^z*-axis. The pseudorapidity is defined in terms of the polar angle θ as $\eta = -\ln \tan(\theta/2)$. Angular distance is measured in units of $\Delta R = \sqrt{(\Delta y)^2 + (\Delta \phi)^2}$.

were applied to the simulated events so that the particle candidates' selection efficiencies, energy scales and energy resolutions match those determined from data control samples. The simulated samples are normalised to their cross sections, and generated to the highest order available in perturbation theory.

Samples used to model the g2HDM signal were generated at leading-order (LO) in QCD with Mapgraph v2.9.3 [\[76\]](#page-39-1) with the NNPDF3.1nlo [\[77\]](#page-39-2) parton distribution function (PDF) set. The ATLAS Fast Simulation was used for masses in the range of 200 GeV to 1 TeV with a 100 GeV step. All signals were produced with the set of couplings $\rho_{tt} = \rho_{tc} = \rho_{tu} = 0.1$ $\rho_{tt} = \rho_{tc} = \rho_{tu} = 0.1$. Each signal process described in Section 1 was generated as a separate MC sample. The cross section obtained from the LO generator is used for the normalisation of the signals. Simulated events for different coupling values are obtained by rescaling the samples to match the target cross section and branching ratio of each subprocess. For a given choice of couplings all the processes are taken into account and rescaled. The RPV SUSY signal samples were generated with Madgraph v2.9.3, with up to two extra jets at LO in QCD. The matching scale is set at 1/4 of the mass of the SUSY particle being produced. Supersymmetric particle decays via the RPV coupling are simulated with 25% branching ratio to $\mu/\tau/\nu_{\mu}/\nu_{\tau}$ each, a *b*-quark, and a *b*- or top-quark depending on the lepton charge. The identical branching ratio to second- and third-generation leptons follows from the choice of $\lambda'_{233} = \lambda'_{333}$, while the balance in charged and neutral leptons originates from
the presence of a left-handed lepton superfield in the *LOD* coupling. All signal events were showered with the presence of a left-handed lepton superfield in the $LQ\bar{D}$ coupling. All signal events were showered with Pythia 8.245 [\[72\]](#page-38-10) using the NNPDF2.3lo [\[78\]](#page-39-3) PDF set.

The sample used to model the *tt^{TW}* ($t\bar{t}Z/\gamma^*$) background was generated using SHERPA-2.2.10 [\[79\]](#page-39-4) (SHERPA-2.2.11) where the matrix element (ME) was calculated for up to one (zero) additional parton at next-to-2.2.11), where the matrix element (ME) was calculated for up to one (zero) additional parton at next-toleading-order (NLO) in QCD and up to two partons at LO in QCD using Comix [\[80\]](#page-39-5) and OpenLoops [\[81\]](#page-39-6) and merged with the Sherpa parton shower (PS) [\[82\]](#page-39-7) using the MePs@Nlo prescription [\[83\]](#page-39-8), with a CKKW merging scale of 30 GeV for the $t\bar{t}W$ sample. These samples are generated using the NNPDF3.0nnlo [\[84\]](#page-39-9) PDF set. Both the factorisation and renormalisation scales are set to $\mu_r = \mu_f = m_T/2$ in the *ttW* sample, where m_T is defined as the scalar sum of the transverse masses $\sqrt{m^2 + p_T^2}$ $T_T²$ of the particles generated from the ME calculation. The LO $t\bar{t}W$ electroweak (EW) contributions are obtained from a dedicated sample simulated with SHERPA-2.2.10. The invariant mass of the lepton pair $(m_{\ell^+\ell^-})$ in the $t\bar{t}Z/\gamma^*$
sample is set to be greater than 1 GeV. The complete $t\bar{t}W$ simulation is pormalised to the total cross sample is set to be greater than 1 GeV. The complete $t\bar{t}W$ simulation is normalised to the total cross section of $\sigma(t\bar{t}W) = 614.7$ fb that comes from the SHERPA configuration outlined above considering NLO QCD and NLO EWK effects, based on a similar strategy as used in Ref. [\[85\]](#page-39-10). The $t\bar{t}Z/\gamma^*$ sample is
pormalised to the cross section $\sigma(t\bar{t}Z/\gamma^*) = 830$ fb, calculated at NLO OCD and NLO EW accuracy using normalised to the cross section $\sigma(t\bar{t}Z/\gamma^*) = 839$ fb, calculated at NLO QCD and NLO EW accuracy using
MADGRAPUS, AMC@NLO [86] and scaled by an off shall correction estimated at one loop layel in α MADGRAPH5_AMC@NLO [\[86\]](#page-39-11) and scaled by an off-shell correction estimated at one-loop level in α_s .

The production of $t\bar{t}t\bar{t}$ events was modelled using the MADGRAPH5_aMC@NLO v2.6.2 generator which provides matrix elements at NLO in QCD with the NNPDF3.1nlo. The functional form of the renormalisation and factorisation scales are set to $\mu_r = \mu_f = m_T/4$. Top quarks are decayed at LO using MadSpin to preserve all spin correlations. The events are interfaced with Pythia 8.230 for the parton shower and hadronisation, using the NNPDF2.3lo PDF set. The production of $\tilde{t}\tilde{t}\tilde{t}\tilde{t}$ events is normalised to a cross-section of 12 fb computed at NLO in QCD including EW corrections [\[87\]](#page-39-12).

Diboson (*VV*) background processes are simulated with Sherpa 2.2.2 [\[79\]](#page-39-4). The matrix element was calculated using Comix [\[80\]](#page-39-5) and OpenLoops [\[81\]](#page-39-6) with NLO accuracy in QCD for up to one additional parton and at LO accuracy for up to three additional partons, and merged with the SHERPA using MEPs@NLO prescription [\[83\]](#page-39-8). The NNPDF3.0_{NNLO} set of PDFs was used, along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors. The cross section of $\sigma(VV) = 104$ pb was computed by Sherpa 2.2.2.

Samples for $t\bar{t}H$, $t\bar{t}$, and single top production were generated using the NLO generator Powheg-Boxv2 [\[88–](#page-39-13)[93\]](#page-40-0) and interfaced with Pythia 8 for the parton showering and fragmentation. These samples used the NNPDF3.0nlo PDF set. The h_{damp} parameter, which controls the transverse momentum of the first additional emission beyond the LO Feynman diagram in the PS and therefore regulates the high- p_T radiation, is set to $3/4 \times (m_t + m_{\bar{t}} + m_H)$ in the *t*_IH sample and to $1.5 \times m_t$ in the *t*_I and single top samples, where m_t (m_H) denotes the mass of the top quark (SM Higgs boson).

A dedicated *tt*^{\bar{t}} sample including rare $t \to Wb\gamma^*(\to l^+l^-)$ radiative decays, $t\bar{t} \to W^+bW^-\bar{b}l^+l^-$, is generated using a ME calculated at LO in OCD and requiring $m_{\text{min}} > 1$ GeV. In this sample the photon c using a ME calculated at LO in QCD and requiring $m_{\ell^+\ell^-} > 1$ GeV. In this sample the photon can be radiated from the top quark, the W boson or the h-quark. Both the $t\bar{t}Z/v^*$ and $t\bar{t} \rightarrow W^+bW^-\bar{b}l^+l^-$ samples radiated from the top quark, the *W* boson, or the *b*-quark. Both the $t\bar{t}Z/\gamma^*$ and $t\bar{t} \to W^+bW^-\bar{b}l^+l^-$ samples
are combined and together form the " $t\bar{t}Z$ " (bigh mass)" sample. The contribution from interna are combined and together form the " $t\bar{t}Z$ (high mass)" sample. The contribution from internal photon conversions ($\gamma^* \to l^+l^-$) with $m_{\ell^+\ell^-} < 1$ GeV are modelled by QED multiphoton radiation via the PS
in an inclusive $t\bar{t}$ sample and is referred to as " $t\bar{t}\alpha^*$ " (low mass)". Dedicated Z+iets samples containing in an inclusive *tt* sample and is referred to as "*tt*_γ^{*} (low mass)". Dedicated *Z*+jets samples containing
electrons from material photon conversion ($\alpha \rightarrow e^+e^-$) or internal photon conversion are generated with electrons from material photon conversion ($\gamma \to e^+e^-$) or internal photon conversion are generated with
Powyrec-Box and interfaced with Pyrum 8 for the parton showering and fragmentation. These samples Powheg-Box and interfaced with Pythia 8 for the parton showering and fragmentation. These samples are used to model the data in control regions enriched in material and internal conversion electrons, as explained in Section [5.](#page-9-0)

The remaining rare background contributions listed in Table [1](#page-6-0) are normalised using their NLO theoretical cross sections, except for the $t\bar{t}t$, $t\bar{t}W^+W^-$, $t\bar{t}ZZ$, $t\bar{t}HH$, and $t\bar{t}WH$ processes, for which a LO cross section is used.

Table 1: The configurations used for event generation of signal and background processes. The samples used to estimate the systematic uncertainties are indicated in parentheses and grey. *V* refers to production of an electroweak boson (*W* or Z/γ^*). The matrix element order refers to the order in the strong coupling constant of the perturbative calculation. The "*tTW* (FW)" sample also includes next-to-leading-order electroweak corrections. Th calculation. The " $t\bar{t}W$ (EW)" sample also includes next-to-leading-order electroweak corrections. Tune refers to the underlying-event tune of the parton shower generator. MG5_aMC refers to MadGraph5_aMC@NLO 2.2, 2.3, or 2.6; Рутниа 6 refers to version 6.427 [\[94\]](#page-40-1); Рутниа 8 refers to version 8.2; MEPs@NLo refers to the method used in SHERPA to match the matrix element to the parton shower. All samples include leading-logarithm photon emission, either modelled by the parton shower generator or by Photos [\[95\]](#page-40-2). The mass of the top quark (m_t) and SM Higgs boson were set to ¹⁷².⁵ GeV and ¹²⁵ GeV, respectively.

Process	Generator	ME order	Parton shower PDF		Tune
g2HDM signal	MG5_aMC	LO	PYTHIA ₈	NNPDF3.1nlo	A14
SUSY signal	MG5_aMC	LO	PYTHIA ₈	NNPDF3.1nlo	A14
$t\bar{t}W$	SHERPA 2.2.10	MEPs@NLO	SHERPA	NNPDF3.0nnlo	SHERPA default
	$(MG5_aMC)$	(NLO)	(PYTHIA 8)	(NNPDF3.0nlo)	(A14)
$t\bar{t}W$ (EW)	SHERPA 2.2.10	LO	SHERPA	NNPDF3.0nnlo	SHERPA default
	$(MG5_aMC)$	(LO)	(PYTHIA 8)	(NNPDF3.0nlo)	(A14)
$t\bar{t}t\bar{t}$	MG5_aMC	NLO	PYTHIA ₈	NNPDF3.1nlo	A14
	(SHERPA 2.2.10) (MEPS@NLO) (SHERPA)				(NNPDF3.0nnlo) (SHERPA default)
$t\overline{t}H$	POWHEG-BOX	NLO	PYTHIA ₈	NNPDF3.0nlo	A14
	(POWHEG-BOX) (NLO)			(HERWIG7.0.4) (NNPDF3.0nlo)	(H7-UE-MMHT)
	$(MG5_aMC)$	(NLO)	(PYTHIA 8)	(NNPDF3.0nlo)	(A14)
$t\bar{t}(Z/\gamma^* \to l^+l^-)$	SHERPA 2.2.11	MEPs@NLo	SHERPA	NNPDF3.0nnlo	SHERPA default
	$(MG5_aMC)$	(NLO)	(PYTHIA 8)	(NNPDF3.0nlo)	(A14)
$t\bar{t} \rightarrow W^{+}bW^{-}\bar{b}l^{+}l^{-}$	MG5_aMC	LO	PYTHIA ₈	NNPDF3.01o	A14
$t(Z/\gamma^*)$	MG5_aMC	NLO	PYTHIA ₈	NNPDF2.31o	A14
$tW(Z/\gamma^*)$	MG5_aMC	NLO	PYTHIA ₈	NNPDF2.31o	A14
tt	POWHEG-BOX	NLO	PYTHIA ₈	NNPDF3.0nlo	A14
	(POWHEG-BOX) NLO			(HERWIG7.1.3) (NNPDF3.0nlo)	(H7-UE-MMHT)
$t\bar{t}$	MG5_aMC	LO	PYTHIA ₈	NNPDF2.31o	A14
Single top	POWHEG-BOX	NLO	PYTHIA ₈	NNPDF3.0nlo	A14
$(t-$, $Wt-$, s -channel)					
VV, qqVV, VVV	SHERPA 2.2.2	MEPs@NLO	SHERPA	NNPDF3.0nnlo	SHERPA default
$Z \rightarrow l^+l^-$	SHERPA 2.2.1	MEPs@NLO	SHERPA	NNPDF3.0nlo	SHERPA default
$Z \rightarrow l^+l^-(\gamma \rightarrow e^+e^-)$ Powheg-BOX		NLO	PYTHIA ₈	CTEQ6L1nlo	A14
$Z \rightarrow l^+l^-(\gamma^* \rightarrow e^+e^-)$ Powheg-BOX		NLO	PYTHIA ₈	CTEQ6L1nlo	A14
$W+{\rm jets}$	SHERPA 2.2.1	MEPs@NLo	SHERPA	NNPDF3.0nlo	SHERPA default
VH	POWHEG-BOX	NLO	PYTHIA ₈	NNPDF3.0nlo	A14
$t\bar{t}W^+W^-$	MG5_aMC	LO	PYTHIA ₈	NNPDF2.3lo	A14
$t\overline{t}ZZ$	$MG5$ _{_a} MC	LO	PYTHIA ₈	NNPDF2.3lo	A14
ttHH	MG5_aMC	LO	PYTHIA ₈	NNPDF2.31o	A14
$t\bar{t}WH$	MG5_aMC	LO	PYTHIA ₈	NNPDF2.31o	A14

4 Event reconstruction and object identification

Interaction vertices from the *pp* collisions are reconstructed from at least two tracks with transverse momentum (p_T) larger than 500 MeV that are consistent with originating from the beam collision region in the $x - y$ plane. If more than one primary vertex candidate is found in the event, the candidate for which the associated tracks form the largest sum of squared p_T is selected as the hard-scatter primary vertex [\[96\]](#page-40-3).

Electron candidates are reconstructed from energy clusters in the electromagnetic calorimeter matched to a track in the ID [\[97\]](#page-40-4). They are required to satisfy $p_T > 10$ GeV and $|\eta_{\text{cluster}}| < 2.47$, excluding the transition region between the endcap and barrel calorimeters (1.37 $\langle \eta_{\text{cluster}} \rangle$ < 1.52). Loose and tight electron identification working points are used [\[97\]](#page-40-4), based on a likelihood discriminant employing calorimeter, tracking and combined variables that provide separation between electrons and jets. The associated track of an electron candidate is required to have at least two hits in the pixel detector and seven hits total in the pixel and silicon-strip detectors combined. For the tight identification working point, one of these pixel hits must be in the innermost layer, or the next-to-innermost layer if the module traversed in the innermost layer is non-operational, and there must be no association with a vertex from a reconstructed photon conversion [\[98\]](#page-40-5) in the detector material (denoted as 'material conversion' in this paper).

Muon candidates are reconstructed by combining tracks in the ID with tracks in the MS [\[99\]](#page-40-6). The resulting muon candidates are re-fit using the complete track information from both detector systems [\[100\]](#page-40-7). They are required to satisfy $p_T > 10$ GeV and $|\eta| < 2.5$. Loose and medium muon identification working points are used [\[100\]](#page-40-7).

Electron (muon) candidates are matched to the primary vertex by requiring that their longitudinal impact parameter, z_0 , satisfies $|z_0 \sin \theta|$ < 0.5 mm, where θ is the polar angle of the track, and requiring that the significance of their transverse impact parameter, d_0 , satisfies $|d_0/\sigma(d_0)| < 5(3)$, where $\sigma(d_0)$ is the measured uncertainty in d_0 .

To further suppress leptons from heavy-flavour hadron decays, misidentified jets, or photon conversions (collectively referred to as 'non-prompt leptons'), lepton candidates are also required to be isolated in the tracker and in the calorimeter. A track-based lepton isolation criterion is defined by calculating the quantity $I_R = \sum p_T^{\text{trk}}$, where the scalar sum includes all tracks (excluding the lepton candidate itself) within the cone defined by [∆]*^R* < *^R*cut around the direction of the lepton. The value of *^R*cut is the smaller of *^r*min and 10 GeV/ p_T^{ℓ} , where r_{\min} is set to 0.2 (0.3) for electron (muon) candidates and where p_T^{ℓ} is the lepton p_T . All lepton candidates must satisfy $I_R/p_T^{\ell} < 0.15$. Additionally, electrons (muons) are required to satisfy a colorimeter-based isolation criterion; the sum of the transverse energy within a cone of size $\Delta R = 0.2$ calorimeter-based isolation criterion: the sum of the transverse energy within a cone of size $\Delta R = 0.2$ around the lepton, after subtracting the contributions from pile-up and the energy deposit of the lepton itself, is required to be less than 20% (30%) of p_T^{ℓ} . Muons are required to be separated by $\Delta R > 0.2$ from
any selected jets (defined below). If two electrons are closer than $\Delta R = 0.1$ only the one with the higher any selected jets (defined below). If two electrons are closer than $\Delta R = 0.1$, only the one with the higher *p*T is considered. Electrons within $\Delta R = 0.1$ of a selected muon are removed.

The selection criteria described above greatly suppress the contribution from non-prompt leptons. However, several channels considered in this search have additional suppression requirements targeting the main non-prompt lepton types. Non-prompt leptons from hadron decays that contain bottom- and charm-quarks, denoted as 'heavy-flavour (HF) non-prompt leptons', are further rejected using a boosted decision tree (BDT) discriminant, referred to as the non-prompt lepton BDT [\[101\]](#page-40-8), that uses isolation and lifetime information associated with a track jet that matches the selected light lepton. Three working points (WPs) are used: *Tight*, *VeryTight*, and *Tight-not-VeryTight*. The first two provide a selection of prompt-like leptons with an efficiency for muons (electrons) that satisfy the calorimeter- and track-based isolation

Table 2: Description of the loose inclusive ("*L*"), medium inclusive ("*M*"), medium exclusive ("*M*ex"), and tight (" T ") lepton definitions. The electron e^* is required to fulfil, in addition to the corresponding lepton definition requirements, those corresponding to an internal or material conversion candidate.

	e				μ			
	L	M	$M_{\rm ex}$.,	M	$M_{\rm ex}$	
Isolation	Yes			Yes				
Non-prompt lepton BDT WP	Tight VeryTight Tight-not- No		N _o	Tight	Tight-not-	VeryTight		
			VeryTight				VeryTight	
Identification	Loose		Tight		Loose	Medium		
Electron charge-misassignment veto	No		Yes		N/A			
Electron conversion candidate veto	No	Yes (except e^*)			N/A			
Transverse impact parameter	< 5			$<$ 3				
significance $ d_0 /\sigma_{d_0}$								
Longitudinal impact parameter	< 0.5 mm							
$ z_0 \sin \theta $								

criteria of about 50% (70%) for *p*^T ∼ 20 GeV and reaches a plateau of 90% at *p*^T ∼ 55 (50) GeV. The corresponding rejection factor^{[2](#page-8-0)} against leptons from the decay of *b*-hadrons ranges from 29 to 50 (6 to 18) depending on the p_T and η , after resolving ambiguities between overlapping reconstructed objects. The latter allows to select non-prompt-like leptons and is part of the event selection of the control regions enriched in HF non-prompt lepton background, as described in Section [6.](#page-16-0)

In order to further suppress electrons with incorrect charge assignment, a BDT discriminant based on calorimeter and tracking quantities [\[102\]](#page-40-9) is used. An efficiency of 88% for isolated electrons with correct charge assignment is obtained, with a rejection factor of ∼3.3 for isolated electrons with incorrect charge assignment. Material and internal conversion candidates are identified based on a combination of requirements on the invariant mass of tracks and the radius from the reconstructed displaced vertex to the primary vertex. Material conversion candidates have a reconstructed displaced vertex with radius $r > 20$ mm that includes the track associated with the electron.^{[3](#page-8-1)} The invariant mass of the associated track and the closest (in $\Delta \eta$) opposite-charge track reconstructed in the silicon detector, calculated at the conversion vertex, is required to be < ¹⁰⁰ MeV. Internal conversion candidates, which correspond to the internal photon conversions (see Section [3\)](#page-3-1), are required to fail the requirements for material conversions, and the di-track invariant mass, calculated here at the primary vertex, is also required to be < 100 MeV.

The various lepton working points used in this analysis are summarised in Table [2.](#page-8-2) After the initial categorisation based on loose leptons (corresponding to "L"), the most optimal lepton working point to further optimise the event selection is chosen depending on the main background processes and the number of expected events in each category. The various choices can be seen for the signal and control regions in Section [5.](#page-9-0) All *M*, M_{ex} , and *T* electrons in the analysis are required to not be material nor internal conversion candidates, with the exception of the electron in the control regions enriched with internal and material conversions. Those electrons must be an internal or material conversion candidate, respectively, and is denoted as e^* , regardless of the conversion mechanism (see Section [5\)](#page-9-0).

The constituents for jet reconstruction are identified by combining measurements from both the ID and the calorimeter using a particle flow (PFlow) algorithm [\[103,](#page-40-10) [104\]](#page-40-11). Jet candidates are reconstructed from

² The rejection factor is defined as the reciprocal of the efficiency.

³ The beampipe and insertable B-layer inner radii are 23.5 mm and 33 mm, respectively.

these PFlow objects using the anti- k_t algorithm [\[105,](#page-40-12) [106\]](#page-40-13) with a radius parameter of $R = 0.4$. They are calibrated using simulation with corrections obtained from in situ techniques in data [\[104\]](#page-40-11). Only jet candidates with a $p_T > 25$ GeV and within $|\eta| < 2.5$ are selected. In order to reduce the effect from pile-up, each jet with $p_T < 60$ GeV and $|\eta| < 2.4$ is required to satisfy the "Tight" working point of the Jet Vertex Tagger (JVT) [\[107\]](#page-41-0) criteria used to identify the jets as originating from the selected primary vertex. A set of quality criteria is also applied to reject events containing at least one jet arising from non-collision sources or detector noise [\[108\]](#page-41-1).

Jets containing *b*-hadrons are identified (*b*-tagged) via the DL1r algorithm [\[109,](#page-41-2) [110\]](#page-41-3) that uses a deeplearning neural network based on the distinctive features of the *b*-hadrons in terms of the impact parameters of tracks and the displaced vertices reconstructed in the ID. Additional input to this network is provided by discriminant variables constructed by a recurrent neural network [\[111\]](#page-41-4), which exploits the spatial and kinematic correlations between tracks originating from the same *b*-hadron. For each jet, a value for the multivariate *b*-tagging discriminant is calculated. A jet is *b*-tagged if the *b*-tagging score is above a certain threshold, referred to as a working point (WP). Four WPs are defined with average expected efficiencies for *b*-jets of 60%, 70%, 77% and 85%, as determined in simulated $t\bar{t}$ events. The *b*-tagging distribution obtained by ordering the resulting five exclusive bins from the four WPs from higher to lower *b*-jet efficiency is referred to as "pseudo-continuous" *b*-tagging score, and it is used as input to the multivariate analysis discriminant described in Section [5.](#page-9-0) In this search, a jet is considered *b*-tagged if it passes the WP corresponding to 77% or 60% efficiency to tag a b-jet, with a light-jet^{[4](#page-9-1)} rejection factor of about 192 or 2500, and a charm-jet (*c*-jet) rejection factor of about 6 or 40, as determined for jets with $p_T > 20$ GeV and $|\eta| < 2.5$ in simulated *tt* events. Correction factors derived from dedicated calibration samples enriched in *b*-jets, *c*-jets, or light jets, are applied to the simulated samples [\[109,](#page-41-2) [112,](#page-41-5) [113\]](#page-41-6). The notation $b^{77\%}$ and $b^{60\%}$ is used to denote the number of *b*-tagged jets with the corresponding WP.

The missing transverse momentum $\vec{p}_{\rm T}^{\rm miss}$ (with magnitude $E_{\rm T}^{\rm miss}$) is defined as the negative vector sum of the p_T of all selected and calibrated objects in the event, including a term to account for the momentum from soft particles in the event that are not associated with any of the selected objects [\[114\]](#page-41-7). This soft term is calculated from inner-detector tracks matched to the selected primary vertex, which makes it more resilient to contamination from pile-up interactions. The E_T^{miss} distribution is used as an input variable to the machine learning training discussed in Section [5.](#page-9-0)

5 Search strategy

Events are required to pass a minimal preselection and are then categorised into orthogonal signal regions based on different criteria such as number of leptons, total lepton charge (indicated by *Q*), and a multi-output deep neural network classifier (*DNN^{cat}*). This categorisation provides a set of regions that are sensitive to all the possible signal production and decay modes considered in this search. A deep neural network is trained in each of the signal regions to discriminate the signal from the backgrounds (*DNN*SB). Additional orthogonal control regions are defined in order to fit the normalisation of the main backgrounds. Dedicated kinematic selections are applied to the control regions in order to improve the purity of the targeted backgrounds. A maximum-likelihood fit is performed across categories in order to test for a possible signal and constrain in-situ the leading backgrounds simultaneously.

⁴ 'Light jet' refers to a jet originating from the hadronisation of a light quark (u, d, s) or a gluon.

Events were selected for read-out using a combination of single-lepton and di-lepton triggers, requiring the electrons or muons to satisfy identification criteria similar to those used in the offline reconstruction and isolation requirements [\[115,](#page-41-8) [116\]](#page-41-9). For the analysis selection, at least two jets and at least two leptons are required in the event, and leptons are required to match, with [∆]*^R* < ⁰.15, the corresponding leptons reconstructed by the trigger and to have a p_T exceeding the trigger p_T threshold by 1 GeV. Events are required to contain at least one *b*-tagged jet with the 60% efficiency working point, or at least two *b*-tagged jets with the 77% efficiency working point. If events contain pairs of opposite-sign charge and same-flavour leptons (OS-SF), all pairs are required to satisfy a mass requirement on the di-lepton system mass of $m_{\ell^+\ell^-}^{OS-SF} > 12$ GeV and $|m_{\ell^+\ell^-}^{OS-SF} - m_Z| > 10$ GeV. Three disjoint event categories are defined according
to the number of loose leptons in the event: same-charge dilepton (2/SS), three-lepton (3/), and four-lepton to the number of loose leptons in the event: same-charge dilepton (2 ℓ SS), three-lepton (3 ℓ), and four-lepton (4 ℓ) categories. Leptons are ordered by n_{min} the 2 ℓ regions. In the 3 ℓ regions the lepton (4 ℓ) categories. Leptons are ordered by p_T in the 2 ℓ SS and 4 ℓ regions. In the 3 ℓ regions the lepton with opposite-sign charge is taken first, followed by the two same-sign leptons in p_T order. The p_T and identification requirements of each lepton in each category are optimised based on a compromise between non-prompt lepton background suppression and signal acceptance enhancement, and are summarised in Table [3.](#page-11-0)

Multiple control regions are defined in order to fit the normalisation of the leading backgrounds. These regions are orthogonal to the signal regions and with one another based on different requirements on the lepton working points, dilepton invariant mass, and jet and *b*-jet multiplicities. Two regions enriched in diboson and *t* \overline{tZ} are defined by requiring one OS-SF pair compatible with a *Z*-boson, $|m_{\ell+\ell^-}^{OS-SF} - m_Z| < 10$
GeV differing in the jet multiplicity requirement. Two control regions enriched in photon conversions f GeV, differing in the jet multiplicity requirement. Two control regions enriched in photon conversions from $Z \rightarrow \mu \mu \gamma^* (\rightarrow ee)$ are defined, according to the identification of the electron as a material conversion or μ internal conversion candidate. Finally, six control regions are defined enriched in HE non-prompt leptons internal conversion candidate. Finally, six control regions are defined enriched in HF non-prompt leptons, making use of the exclusive lepton identification *M*ex in order to be orthogonal to the signal regions. Events with two same-sign leptons are split according to the criteria (T, M_{ex}) , (M_{ex}, T) , (M_{ex}, M_{ex}) for the leading and subleading leptons in p_T , and further split according to the subleading lepton flavour. This splitting creates six control regions sensitive to different relative composition of electron and muon non-prompt lepton backgrounds. Additionally, the transverse mass of the leading lepton and the missing transverse energy, $m_T(\ell_0, E_T^{\text{miss}})$, defined as $\sqrt{2 \times E_T^{\text{miss}} \times p_{T,\ell_0} \times (1 - \cos(\phi_{miss} - \phi_{\ell_0}))}$, is required to be lower than 250 GeV in the (T, M_{ex}) and (M_{ex}, T) regions, in order to reduce the $t\bar{t}W$ contribution in these CRs. The full definition of the kinematic selection applied to each control region is given in Table [4.](#page-12-0) Figure [3](#page-13-0) illustrates the categorisation and definition of the signal and control regions being fit simultaneously in this analysis. The signal contamination is found to be at most 3% of the total prediction in the control regions, assuming m_H =400 GeV and $\rho_{tt} = 0.4$, $\rho_{tc} = 0.2$, and $\rho_{tu} = 0.2$.

In order to better target each of the possible signals, a *DNN^{cat}* is trained to identify each of the five possible production and decay modes of the g2HDM signal. Two DNN^{cat} are trained individually for the 2ℓ SS and 3ℓ channels using the KERAS library [\[117\]](#page-41-10) with TENSORFLOW as a backend [\[118\]](#page-41-11) and Adam optimiser [\[119\]](#page-41-12). Hyperparameters are optimised with the Talos library [\[120\]](#page-41-13). The networks consist of nine input features, two dense fully-connected layers of 33 nodes with rectified linear units as activation functions, interleaved with a drop-out layer with 20% rate, and five (three) output nodes with a soft-max activation function for the categorisation of $2\ell SS$ (3 ℓ) events. The output categories correspond to the five production modes considered, ignoring in the 3ℓ category signals that can not produce three leptons. Each event is categorised according to the highest class probability. The nine input features are the number of jets, *b*-tagging score of the three leading jets, sum of *b*-tagging score of all jets, sum of all pair-wise angular distances between leptons, scalar sum of jet p_T , scalar sum of lepton p_T , and the event E_T^{miss} . The network is trained with batch size of 2000 and up to 100 epochs, using all the available signal mass points. To avoid discarding

Table 3: Event selection summary in the signal regions. Leptons are ordered by p_T in the 2 ℓ SS and 4 ℓ regions. In the 3ℓ regions the lepton with opposite-sign charge is taken first, followed by the two same-sign leptons in p_T order. In the lepton selection, *T, M, L* stand for Tight, Medium and Loose lepton definitions. In the region naming, the "CAT ttX" denotes the category based on the *DNN*cat output enriched in the signal process "ttX". Each of these regions is split according to the lepton charge of the same-sign lepton pair ("++" or "- -").

Lepton category	2ℓ SS	3ℓ	4ℓ			
Lepton definition	(T, T) with ≥ 1 $b^{60\%}$ (T, M) with ≥ 2 $b^{77\%}$	(L, T, M) with ≥ 1 $b^{60\%}$ (L, M, M) with ≥ 2 $b^{77\%}$	(L, L, L, L)			
Lepton p_T [GeV]	(20, 20)	(10, 20, 20)	(10, 10, 10, 10)			
$m_{\ell^+ \ell^-}^{OS-SF}$ [GeV]		>12				
$ m_{f^+f^-}^{OS-SF} - m_Z $ [GeV]		>10				
N_{jets}						
$N_{b-{\rm jets}}$	≥ 1 $b^{60\%}$ ≥ 2 $b^{77\%}$					
Region split	(sstt, ttq, ttt, tttq, tttt) $\times (Q^{++}, Q^{--})$	(ttt, tttq, tttt) $\times (Q^+,Q^-)$				
Region naming	$2\ell SS$ ++ CAT sstt	3ℓ ++ CAT ttt	4ℓ			
	$2\ell SS$ ++ CAT ttq	$3\ell +$ CAT tttq				
	$2\ell SS$ ++ CAT ttt	3ℓ ++ CAT tttt				
	$2\ell SS$ ++ CAT tttq	3ℓ - CAT ttt				
	$2\ell SS$ ++ CAT tttt	3ℓ -- CAT tttq				
	2ℓ SS $--$ CAT sstt	3ℓ -- CAT tttt				
	2ℓ SS $--$ CAT ttq					
	$2\ell SS$ -- CAT ttt					
	2ℓ SS $-$ CAT tttq					
	$2\ell SS$ -- CAT tttt					

signal events in the evaluation, cross-training is used with the events divided by even/odd event number.

Since several of the probed signal processes are expected to be charge-asymmetric, all the 2 ℓ SS and 3 ℓ regions are further split into two categories each corresponding to the positive and negative total lepton charge selections. Figures $4(a)$ and $4(b)$ show the normalized distributions of the targeted signals with a scalar mass of 400 GeV or 1000 GeV, compared to the expected background distribution across the various categories described in Table [3.](#page-11-0) At high signal mass, a strong migration is observed from the ttt to the tttq category, due to the high probability of additional radiation. Figures $4(c)$ and $4(d)$ show the expected fractional signal contribution in each category for the benchmark coupling. The signals originating from top-Higgs associated production (ttq and ttt) are expected to dominate across all regions, including the categories designed to target other processes, due to the much larger production cross section. This contribution is however strongly dependent on the coupling choice. For the benchmark coupling of $\rho_{tt} = 0.4$, $\rho_{tc} = 0.2$, $\rho_{tu} = 0.2$, the decay to top-quark pairs dominates when not suppressed by the

Table 4: Event selection summary in the control regions. The notation e^* is used to denote material conversion or internal conversion candidates, as described in Section [4.](#page-7-0) In the HF non-prompt lepton region naming, " $2\ell SStt(e)$ " (" $2\ell SStt(\mu)$ ") refer to the control regions enriched in non-prompt electrons (muons) from semileptonic *b*-decays originating mostly from $t\bar{t}$ and with the lepton flavours for the leading and subleading leptons corresponding to "*ee*, μe " (" $\mu\mu$, $e\mu$ "). The additional (*T*, M_{ex}), (M_{ex} , *T*), and (M_{ex} , M_{ex}) subscripts refer to the lepton definitions required for the leading and subleading leptons in each region.

Control regions	WZ	$t\bar{t}Z$	Conversions	HF non-prompt		
N_{jets}	2 or 3	≥ 4	≥ 0	≥ 2		
$N_{b-{\rm jets}}$		≥ 1 $b^{60\%}$ $\parallel \geq 2$ $b^{77\%}$	$0 h^{77\%}$	$1 h^{77\%}$		
Lepton requirement	3ℓ		$\mu\mu e^*$	2ℓ SS		
Lepton definition	(L, M, M)			$(T, M_{\rm ex}) \parallel (M_{\rm ex}, T) \parallel (M_{\rm ex}, M_{\rm ex})$		
Lepton p_T [GeV]	(10, 20, 20)			(20, 20)		
$m_{\ell+\ell-}^{OS-SF}$ [GeV]		>12	>12			
$ m_{\ell+\ell-}^{OS-SF} - m_Z $ [GeV]		<10	>10			
$ m_{\ell\ell\ell} - m_Z $ [GeV]			~10			
$m_T(\ell_0, E_T^{\text{miss}})$ [GeV]				< 250		
Region split			internal / material	subleading $e/\mu \times [(T, M_{\rm ex}), (M_{\rm ex}, T), (M_{\rm ex}, M_{\rm ex})]$		
Region naming	3ℓ VV	3ℓ tt Z	$3\ell Int C$	2ℓ tt(e) _{(T,Mex}), 2ℓ tt(e) _(Mex,T) , 2ℓ tt(e) _{(Mex,Mex})		
			3ℓ MatC	2ℓ tt $(\mu)_{(T,M_{\rm ex})}, 2\ell$ tt $(\mu)_{(M_{\rm ex},T)}, 2\ell$ tt $(\mu)_{(M_{\rm ex},M_{\rm ex})}$		

Table 5: Input variables to the training of the *DNN^{cat}* and *DNN^{SB}* discriminants.

available phase-space.

A total of 27 analysis regions are defined, with 17 signal regions (10 with 2 ℓ SS, 6 with 3 ℓ , and one 4 ℓ) and 10 control regions. In each region, a given kinematic variable is fit to improve the sensitivity to the targeted signal process (signal regions) or to improve the modelling of a particular background process (control regions).

A *DNN*SB classifier is trained in each signal region to separate the targeted signal from the sum of backgrounds. The networks consist of 12 input features, two dense fully-connected layers of 36 and 48 nodes respectively with sigmoid activation functions, interleaved with a drop-out layer with 40% rate,

Figure 3: Illustrative sketch of the definition of the signal and control regions. At the bottom of each region box the corresponding observable used in the simultaneous fit as described in Section [8](#page-22-0) is shown.

and one output node with a sigmoid activation function. The 12 input features are the leading jet p_T , number of muons, transverse mass of leading lepton and E_T^{miss} system, and the nine variables that are used in the *DNN^{cat}*. Table [5](#page-12-1) summarises the input variables used for each multivariate discriminant. In order to achieve good sensitivity over the large range of masses that are tested, the output of the classifier is decorrelated from the signal mass introducing an additional term to the loss function via distance correlation [\[121,](#page-41-14) [122\]](#page-41-15). A hyperparameter λ controls the weight of the additional penalty term, with a value of $\lambda = 0.5$. The value was optimised to achieve a minimal signal mass dependence without compromising the discrimination power. A separate training is performed in each lepton category and signal category. The same *DNN*SB is used in both positive- and negative-charge regions. Figure [5](#page-15-0) shows the *DNN*SB distribution of the targeted signal in each signal-enriched category, the total signal, and the background in the $2\ell SS$ ++ CAT sstt, $2\ell SS$ ++ CAT ttq, 3ℓ ++ CAT ttt, 3ℓ ++ CAT tttq, 3ℓ ++ CAT tttt, and 4 ℓ categories.

In the diboson and *tt*Z control regions the fitted variable is *N*_{b−jets}, where the distribution is binned with an upper limit of ≥ 2 *b*-jets and ≥ 3 *b*-jets respectively. The subleading lepton p_T spectrum is used in the HF non-prompt control regions. Finally, the total event yield is fit in the control regions enriched in electrons from photon conversion.

Figure 4: Distributions for each signal process category (top row), compared to the total expected background, for (a) 400 GeV and (b) 1000 GeV scalar masses. All distributions are normalised to unity. The vertical dashed grey lines separate categories targeting each of the main signal processes: sstt, ttq, ttt, tttq, and tttt. Signal contributions below 2% in a single bin are omitted for clarity. The expected fractional signal contribution in each category (bottom row) is shown for (c) 400 GeV and (d) 1000 GeV scalar masses for the coupling set $\rho_{tt} = 0.4$, $\rho_{tc} = 0.2$, $\rho_{tu} = 0.2$.

Figure 5: Comparison of the *DNN*^{SB} distribution of the targeted signal (solid line), the total signal (dashed line) and the background (filled grey area) in the (a) 2ℓ SS CAT sstt, (b) 2ℓ SS CAT ttq, (c) 3ℓ CAT ttt, (d) 3ℓ CAT tttq, (e) 3 ℓ CAT tttt, and (f) 4 ℓ categories, for an assumed $m_H = 400$ GeV (pink) and $m_H = 800$ GeV (violet), with couplings $\rho_{tt} = 0.4$ and $\rho_{tq} = 0.2$. All distributions are normalised to unity.

6 Background estimation

The background processes passing the signal region selections are categorised into irreducible and reducible backgrounds. Irreducible backgrounds (Section [6.1\)](#page-16-1) produce prompt leptons in their decay, i.e. originating from W/Z boson decays, leptonic τ -lepton decays, or internal conversions. Reducible backgrounds (Section [6.2\)](#page-18-0) have prompt leptons with misassigned charge or at least one non-prompt lepton.

Except for the background from electrons with misassigned charge (denoted as QMisID), all other backgrounds are estimated using the simulated samples described in Section [3.](#page-3-1) In some cases, the simulation is improved using additional corrections derived from data control samples before the simultaneous fit to data. In particular, the event kinematics of the simulated $t\bar{t}$ and *VV* backgrounds require dedicated corrections to better describe the data. In addition, the yields of some simulated backgrounds, in particular $t\bar{t}W$, $t\bar{t}Z$, *VV* and non-prompt-lepton backgrounds, are adjusted via normalisation factors that are determined by performing a likelihood fit to data across all event categories (signal and control regions as defined in Tables [3](#page-11-0) and [4\)](#page-12-0) as discussed in Section [8.](#page-22-0)

6.1 Irreducible backgrounds

Background contributions with prompt leptons originate from a wide range of physics processes with the relative importance of individual processes varying by channel. The main irreducible backgrounds originate from $t\bar{t}W$, $t\bar{t}t\bar{t}$, and $t\bar{t}Z/\gamma^*$ production, followed by *VV* (in particular *WZ*) and $t\bar{t}H$ production, and have final states and kinematic properties similar to the α ?HDM signal. Smalle and have final states and kinematic properties similar to the g2HDM signal. Smaller contributions originate from the following rare processes: tZ , tW , tWZ , $t\overline{t}WW$, VVV , and $t\overline{t}t$ production.

6.1.1 $t\bar{t}W$ background

The *t*^TW background represents the leading background in several event categories. Despite the use of state-of-the-art simulations, accurate modelling of additional QCD and QED radiation in $t\bar{t}W$ production remains challenging. Given the excellent discriminating power of the *DNN*SB in the signal regions, the events at lower values of the DNN^{SB} score are enriched in and sensitive to the $t\bar{t}W$ background. Additionally, the signal regions in the 2ℓ and 3ℓ categories are split by the sign of the total lepton charge (Q) to better discriminate some g2HDM signal processes and the $t\bar{t}W$ process, which have a large charge asymmetry, from other SM backgrounds that are charge symmetric. This discrimination improves the modelling of this background in the simultaneous fit.

Disagreement between the data and the prefit prediction from the simulation is observed, which is accommodated by an overall normalisation factor that is assigned to the $t\bar{t}W$ background, and which is determined during the likelihood fit. The measured normalisation factor is $\hat{\lambda}_{t\bar{t}W} = 1.50 \pm 0.14$, which is
compatible with that determined in the SM $t\bar{t}t\bar{t}$ analysis [123], and with a previous measurement of compatible with that determined in the SM $t\bar{t}t\bar{t}$ analysis [\[123\]](#page-42-0), and with a previous measurement of the $t\bar{t}W$ production cross section [\[124\]](#page-42-1).

Figure 6: Comparison between data and the background prediction for the distribution of (a) the number of jets in the 3ℓ VV0b region before the *VV* jet multiplicity correction and (b) the number of jets in a 3ℓ region with at least one jet and exactly one *b*-jet defined with the 60% WP after the *VV* jet multiplicity correction. The ratio of the data to the background prediction ("Pred.") is shown in the lower panel. The size of the combined statistical and systematic uncertainty in the background prediction is indicated by the blue hatched band. The last bin in each figure contains the overflow.

6.1.2 *VV* and $t\bar{t}Z/\gamma^*$ backgrounds

The *VV* simulated sample was seen to require additional improvements in the modelling of the jet multiplicity spectrum compared to data. Therefore, a data-driven correction is derived from an inclusive trilepton diboson-enriched region with zero *b*-jets defined with the 85% WP for *b*-jet efficiency and at least one jet (denoted as 3ℓ VV0b region). The events are required to have three leptons passing the same selection as in the 3 ℓ *VV* CR.

Figure $6(a)$ shows the jet multiplicity distribution in the 3 ℓ VV0b region before the correction. After the correction is applied to *VV*, the modelling of the N_{jets} distribution improves significantly in a 3 ℓ region with at least one jet and exactly one *b*-jet defined with the 60% WP, as shown in Figure [6\(b\).](#page-17-1)

The 3ℓ VV and 3ℓ ttZ CRs are used in the likelihood fit to improve the prediction of the background contribution from the *VV* and $t\bar{t}Z/\gamma^*$ processes, respectively. The number of jets and *b*-jets provide good
discrimination between these two processes and are used to build the control regions (number of jets) and discrimination between these two processes and are used to build the control regions (number of jets) and as variables used in the fit (number of *b*-jets). The measured normalisation factors are: $\lambda_{VV} = 0.85 \pm 0.30$ and $\hat{\lambda}_{t\bar{t}Z} = 0.97 \pm 0.19$

Figures [7\(a\)](#page-18-1) and [7\(b\)](#page-18-2) show the *b*-jet multiplicity distribution in the 3ℓ VV and 3ℓ ttZ CRs after the likelihood fit to data.

Figure 7: Comparison between data and the background prediction for the distribution of the *b*-jet multiplicity in the (a) 3ℓ VV and (b) 3ℓ ttZ CRs after the *VV* jet multiplicity correction. The background contributions after the likelihood fit to data ("Post-Fit") under the background-only hypothesis are shown as filled histograms. The ratio of the data to the post-fit background prediction ("Pred.") is shown in the lower panel, separately for post-fit background (black points) and pre-fit background (dashed blue line). The size of the combined statistical and systematic uncertainty in the background prediction is indicated by the blue hatched band. The last bin in each figure contains the overflow.

6.1.3 Other irreducible backgrounds

The rate of the background from internal conversions with $m(e^+e^-) < 1$ GeV is estimated using the
two dedicated CBs (3*F*IntC and 3*FMatC*). The total vield in each category is used in the likelihood fit two dedicated CRs (3ℓ IntC and 3ℓ MatC). The total yield in each category is used in the likelihood fit to determine the normalisation factor: $\hat{\lambda}_e^{\text{Int}C} = 1.06 \pm 0.23$, where the uncertainty is dominated by the statistical uncertainty. statistical uncertainty.

6.2 Reducible backgrounds

6.2.1 Non-prompt leptons

Non-prompt leptons originate from material conversions, heavy-flavour hadron decays, or the improper reconstruction of other particles, with an admixture strongly depending on the lepton quality requirements and varying across event categories. These backgrounds are in general small in all 2ℓ and 3ℓ SRs and thus are estimated from simulation, with the normalisation determined by the likelihood fit. The non-prompt lepton background contribution in the 4ℓ SR is negligible and is therefore taken from simulation without dedicated data-driven corrections. The main contribution to the non-prompt-lepton background is from $t\bar{t}$ production, with much smaller contributions from *V*+jets and single-top-quark processes. The non-prompt leptons in the simulated samples are labelled according to whether they originate from heavy-flavour (HF) or light-flavour (LF) hadron decays, or from a material conversion candidate (Mat. Conv.). The HF category includes leptons from both bottom and charm decays.

Two corrections are applied to the $t\bar{t}$ and the overall non-prompt lepton background simulation before the fit. First, the $t\bar{t}$ + ≥ 1 *b*-jet contribution from simulation is known to be mismodelled and is therefore corrected by a factor of 1.3 as measured by a previous ATLAS analysis sensitive to the in-situ measurement of this contribution in the single- and opposite-sign di-lepton final states $[125]$. This correction is well motivated since the mismodeling of additional b -jets in $t\bar{t}$ is not expected to depend on the presence of additional non-prompt leptons in the event. Second, the shape of the *b*-jet multiplicity in the non-prompt lepton background simulation is corrected to match data in an orthogonal $2\ell SS$ validation region enriched with non-prompt leptons, where one of the leptons is required to pass a looser non-prompt lepton BDT score but not pass the M lepton WP.

Several of the event categories introduced in Section [5](#page-9-0) were designed to be enriched in specific processes and are used to derive normalisation factors to improve their modelling by the simulation. The 3ℓ MatC CR is enriched in material conversions and only the total event yield is used. There are six 2ℓ CRs enriched in contributions from HF non-prompt leptons in *tt*^{$t\bar{t}$} events, i.e. $2\ell t t(e)_{(T,M_{ex})}$, $2\ell t t(e)_{(M_{ex},T)}$, $2\ell t t(e)_{(M_{ex},M_{ex})}$,
 $2\ell t t(u)_{(T,K,x)}$, $2\ell t t(u)_{(M,K,x)}$ and $2\ell t(u)_{(M,K,x)}$. In these CBs, the transverse momentu $2\ell t t(\mu)_{(T,M_{\text{ex}})}, 2\ell t t(\mu)_{(M_{\text{ex}},T)},$ and $2\ell t t(\mu)_{(M_{\text{ex}},M_{\text{ex}})}$. In these CRs, the transverse momentum of the subleading lepton, $p_{T, sub-lead \, lep}$, distribution is used to be able to correct for a possible mismodeling in the p_T of the non-prompt lepton. The event requirement to have at least one M_{ex} lepton provides separation from the irreducible backgrounds, in particular $t\bar{t}W$, and thus increases the sensitivity to the HF non-prompt electron and muon contributions. Normalisation factors for three non-prompt-lepton background contributions are estimated from the likelihood fit. The normalisation factor for HF non-prompt leptons is estimated separately for electrons and muons, λ_e^{had}
determined for the material conversions had had and $\lambda_{\mu}^{\text{had}}$ respectively. An additional normalisation factor is determined for the material conversions background, $\lambda_e^{\text{Mat Conv}}$
 $\hat{\lambda}_{\text{had}} = 1.05 \pm 0.31$ $\hat{\lambda}_{\text{had}} = 0.92 \pm 0.18$ and $\hat{\lambda}_{\text{Mat Conv}} = 1.16 \pm 0.02$ $_{e}^{\text{Mat Conv}}$. The measured normalisation factors are: $\hat{\lambda}_e^{\text{had}} = 1.05 \pm 0.31$, $\hat{\lambda}_\mu^{\text{had}} = 0.92 \pm 0.18$, and $\hat{\lambda}_e^{\text{Mat Conv}} = 1.16 \pm 0.29$, where the uncertainties are dominated by the statistical uncertainty by the statistical uncertainty.

Figures [8\(a\)](#page-20-0) and [8\(b\)](#page-20-1) display the sub-leading lepton p_T distribution in the 2ℓ tt(e)(T, M_{ex}) and 2ℓ tt(μ)(T, M_{ex}) CRs after the likelihood fit to data. As shown in the figures, the purity of HF non-prompt lepton background is 43% and 61%, respectively, which was possible to achieve with the usage of the exclusive *M*ex lepton working point.

6.2.2 Charge misassignment

Backgrounds with leptons with the charge incorrectly assigned affect primarily the 2ℓ channel and predominantly arise from $t\bar{t}$ production, with one electron having undergone a hard bremsstrahlung as well as an asymmetric conversion $(e^{\pm} \to e^{\pm} \gamma^* \to e^{\pm} e^+ e^-)$ or a mismeasured track curvature. The muon charge misassignment rate is negligible in the p_T range relevant to this analysis. The electron charge misassignment rate is measured in data using samples of $Z \rightarrow e^+e^-$ events reconstructed as same-charge pairs and as opposite-charge pairs, with the background subtracted via a sideband method. The charge misassignment rate is parameterised as a function of electron *p*_T and |*n*|, and it varies from about 10⁻⁵ for low-*p*_T electrons (17 < *p*_T < 50 GeV) with $|n|$ < 1.37, to about 3 × 10⁻⁴ for high *p*_T electrons (*p*_T > (17 ≤ *p*_T ≤ 50 GeV) with $|\eta|$ ≤ 1.37, to about 3×10^{-4} for high-*p*_T electrons (*p*_T ≥ 100 GeV) with $1.52 \le |\eta| \le 2$. To estimate the QMisID background in each of the corresponding event categories, the measured charge misassignment rate is then applied to data events satisfying the requirements of the 2ℓ channels, except that the two leptons are required to be of opposite charge.

Figure 8: Comparison between data and the background prediction for the distribution of the transverse momentum of the sub-leading lepton (p_T , sub-lead lep) in (a) the 2ℓ tt(e)(T, M_{ev}) CR and (b) the 2ℓ tt(μ)(T, M_{ev}) CR. The background contributions after the likelihood fit to data ("Post-Fit") under the background-only hypothesis are shown as filled histograms. The ratio of the data to the post-fit background prediction ("Pred.") is shown in the lower panel, separately for post-fit background (black points) and pre-fit background (dashed blue line). The size of the combined statistical and systematic uncertainty in the background prediction is indicated by the blue hatched band. The last bin in each figure contains the overflow.

7 Systematic uncertainties

The signal and background yields in each signal and control region may be affected by several sources of systematic uncertainty, described in the following subsections. Given the low background yields and good signal-to-background separation provided by the final discriminating variable used in the signal-rich event categories, the search sensitivity is determined by the limited number of data events rather than by the systematic uncertainties of the background estimation. The final uncertainty in the background estimate in the SRs is dominated by the uncertainty in the fitted background normalisations, in particular $t\bar{t}W$. A summary of all systematic uncertainties included in the analysis is given in Table [6.](#page-22-1)

7.1 Experimental uncertainties

The uncertainty in the combined 2015–2018 integrated luminosity is 1.7% [\[126\]](#page-42-3), obtained using the LUCID-2 detector [\[127\]](#page-42-4) for the primary luminosity measurements.

Uncertainties associated with the lepton selection arise from the trigger, reconstruction, identification and isolation efficiencies, and lepton momentum scale and resolution [\[97,](#page-40-4) [99,](#page-40-6) [102\]](#page-40-9). Uncertainties associated with the jet selection arise from the jet energy scale (JES), the JVT requirement and the jet energy resolution (JER) [\[104,](#page-40-11) [128\]](#page-42-5).

The efficiency of the flavour-tagging algorithm is measured for each jet flavour using control samples in data and in simulation. From these measurements, correction factors are derived to correct the tagging rates in the simulation [\[109,](#page-41-2) [113,](#page-41-6) [129\]](#page-42-6). These systematic uncertainties are taken as uncorrelated between *b*-jets, *c*-jets, and light-flavour jets. An additional uncertainty is assigned to account for the extrapolation of the *b*-tagging efficiency measurement from the p_T region used to determine the correction factors to regions with higher transverse momentum [\[130\]](#page-42-7). This uncertainty is the leading experimental uncertainty in the analysis.

The treatment of the uncertainties associated with reconstructed objects is common to all analysis channels, and thus these are considered as fully correlated among different analysis regions.

7.2 Theoretical uncertainties

Modelling uncertainties on the main irreducible backgrounds are assessed through comparison with alternative MC samples, as listed in Table [1.](#page-6-0) Additional uncertainties are evaluated from renormalisation and factorisation scale variations by a factor of 0.5 and 2, relative to the nominal scales, for the $t\bar{t}W$, *ttZ*, and diboson samples. An additional 50% uncertainty is assigned to $t\bar{t}W$, $t\bar{t}Z$, and $t\bar{t}$ events with additional heavy-flavour jets. This uncertainty is not applied to diboson events with heavy-flavour since its normalisation is fit from data. The statistical uncertainty on the fitted parameters for the *N*_{iets} *VV* correction is propagated as an uncertainty on the diboson background. The leading theoretical uncertainties arise from $t\bar{t}W$ modelling and additional heavy-flavour uncertainties.

Finally, additional normalisation uncertainties are included for all processes where their normalisation is not obtained from the fit. The $\tilde{t}t\tilde{t}$, $\tilde{t}H$, and tZ processes are assigned an uncertainty of 20% [\[87\]](#page-39-12), 11% [\[86\]](#page-39-11), and 5% [\[131\]](#page-42-8) respectively. A 50% cross section uncertainty is assigned as a conservative estimate to the $t\bar{t}t$, tWZ , $t\bar{t}WW$, and triboson backgrounds, as well as to the additional $t\bar{t}W$ electroweak contribution, which are small backgrounds with low impact on the search.

Uncertainties on the modelling of the signal samples are evaluated through independent variations of the factorisation and renormalisation scales by a factor two. Additional uncertainties due to PDF effects are estimated through an ensemble of eigenvariations of the NNPDF set, and taking the difference to alternative PDF sets [\[132\]](#page-42-9).

7.3 Non-prompt lepton uncertainties

The normalisation of HF non-prompt leptons is obtained from regions including at least one M_{ex} lepton and extrapolated to the signal regions where the same-sign leptons fulfill the *T* or *M* identification requirements. An uncertainty of 20% on the extrapolation from M_{ex} to *T* leptons is applied from the comparison of the relative efficiency between nominal and alternative $t\bar{t}$ MC samples. An additional 50% uncertainty is assigned to events originating from $t\bar{t}$ + $\geq 1b$ and $t\bar{t}$ + $\geq 1c$, decorrelated between flavours. Validation regions with looser lepton requirements and further enriched in non-prompt leptons are defined. A good data/MC agreement is observed in all kinematic variables except for the number of *b*-jets. Based on this disagreement, an *N*b−jets-dependent uncertainty is added to the HF non-prompt background ranging from 6%–40% for 1–3 additional *b*-jets in the non-prompt muon regions, and 10%–80% in the non-prompt electron regions.

Table 6: Sources of systematic uncertainty considered in the analysis. "N" means that the uncertainty is taken as normalisation-only for all processes and channels affected. Some of the systematic uncertainties are split into several components, as indicated by the number in the rightmost column.

The modelling of internal and material conversions is tested in dedicated validation regions with two tight same-sign leptons, requiring one of them to be a conversion candidate. An additional uncertainty of 10% and 50% is assigned to the material and internal conversion backgrounds respectively, evaluated from the data/MC agreement in the validation regions.

A systematic uncertainty of 10–60% is assigned to the background from electrons with misidentified charge. The uncertainty increases with electron p_T and decreases with $|\eta|$. The uncertainty is assessed combining the uncertainties from the measurement of the charge misassignment rate, the difference in rates from varying the m_Z window selection, and the different rates measured in data and $Z \rightarrow ee$ MC.

8 Results

A maximum-likelihood fit is performed on all bins in the 27 signal and control regions considered in this search to simultaneously determine the background and the g2HDM signal yields that are most consistent with the data. The DNN^{SB} is used as the discriminating variable in the signal regions, whereas the $N_{b-{\text{jets}}},$ subleading lepton p_T and event yields are fit in the control regions. The sum of all the g2HDM signal

processes studied here (sstt, ttq, ttt, tttq, tttt) is considered as a single signal template and its acceptance in each category is predicted by the simulation.

The likelihood function $\mathcal{L}(\mu, \vec{\lambda}, \vec{\theta})$ is constructed as a product of Poisson probability terms over all bins considered in the search, and depends on the signal-strength parameter, μ , a multiplicative factor applied to the predicted yield for the g2HDM signal (depending on the coupling configuration ρ_{tt} , ρ_{tc} , ρ_{tu} and on the assumed mass m_H (m_A)), $\vec{\lambda}$, the normalisation factors for several backgrounds (see Section [6\)](#page-16-0), and $\vec{\theta}$, a set of nuisance parameters (NP) encoding systematic uncertainties in the signal and background expectations [\[133\]](#page-42-10). Systematic uncertainties can impact the estimated signal and background rates, the migration of events between categories, and the shape of the fitted distributions; they are summarised in Table [6.](#page-22-1) Both μ and $\vec{\lambda}$ are treated as free parameters in the likelihood fit. The NPs $\vec{\theta}$ allow variations of the expectations for signal and background according to the systematic uncertainties, subject to Gaussian or Poisson constraints in the likelihood fit. Their fitted values represent the deviations from the nominal expectations that globally provide the best fit to the data. Statistical uncertainties in each bin due to the limited size of the simulated samples are taken into account by dedicated parameters using the Beeston–Barlow "lite" technique [\[134\]](#page-42-11).

The test statistic q_{μ} is defined as the profile likelihood ratio: $q_{\mu} = -2 \ln(\mathcal{L}(\mu, \hat{\vec{\lambda}}_{\mu}))$ $(\hat{\vec{\theta}}_{\mu})/\mathcal{L}(\hat{\mu}, \hat{\vec{\lambda}}_{\hat{\mu}},$ is defined as the profile likelihood ratio: $q_{\mu} = -2 \ln(\mathcal{L}(\mu, \hat{\vec{\lambda}}_{\mu}, \hat{\vec{\theta}}_{\mu}) / \mathcal{L}(\hat{\mu}, \hat{\vec{\lambda}}_{\hat{\mu}}, \hat{\vec{\theta}}_{\hat{\mu}}))$, where $\hat{\mu}, \vec{\lambda}_{\hat{\mu}}$ and $\hat{\vec{\theta}}_{\hat{\mu}}$ are the values of the parameters that maximise the likelihood function, and $\hat{\vec{\theta}}_{\mu}$ are the set set of the parameters that maximise the likelihood function for a given value of μ . The test sta values of the parameters that maximise the likelihood function for a given value of μ . The test statistic q_μ is evaluated with the RooFit package [\[135\]](#page-42-12). A related statistic is used to determine the probability that the observed data are incompatible with the background-only hypothesis (i.e. the discovery test) by setting $\mu = 0$ in the profile likelihood ratio (q_0). The *p*-value (referred to as p_0) representing the probability of the data being compatible with the background-only hypothesis is estimated by integrating the distribution of *q*⁰ from background-only pseudo-experiments, approximated using the asymptotic formulae given in Ref. [\[136\]](#page-42-13), above the observed value of q_0 . Some model dependence exists in the estimation of the p_0 , as a given signal scenario needs to be assumed in the calculation of the denominator of q_0 , even if the overall signal normalisation is allowed to float and is fit to data. The observed p_0 is checked for each explored signal scenario. Upper limits on the signal production cross section for each of the signal scenarios considered are derived by using q_μ in the CL_s method [\[137,](#page-42-14) [138\]](#page-43-0). For a given signal scenario, values of the production cross section (parameterised by μ) yielding $CL_s < 0.05$, where CL_s is computed using the asymptotic approximation [136], are excluded at $> 95\%$ confidence level (CL) asymptotic approximation [\[136\]](#page-42-13), are excluded at \geq 95% confidence level (CL).

The smallest p_0 value is observed when assuming a signal with $m_H = 1000$ GeV and (ρ_{tt} =0.32, ρ_{tc} =0.05, and ρ_{tu} =0.85), corresponding to a local significance of 2.81standard deviations. The signal cross section resulting from the fit to data for this g2HDM signal hypothesis is 138 fb, with fractional contributions of 71% ttq, 20% sstt, and 9% ttt. Figure [9](#page-24-0) shows the local significance as a function of the three couplings normalised to the sum of the couplings. This normalisation is performed in order to eliminate one degree of freedom related to the total normalisation of the signal, which is not relevant for the computation of the significance.

A comparison of the distributions of observed and expected yields is shown Figure $10(a)$ for the 17 SRs, and Figure [10\(b\)](#page-25-1) for the 10 CRs, after the combined likelihood fit for the signal-plus-background hypothesis. The corresponding post-fit yields for the SRs can be found in Tables [7,](#page-26-0) [8,](#page-26-1) and [9](#page-27-0) for the 2ℓ SS positively-charged, 2 ℓ SS negatively-charged, and 3 ℓ and 4 ℓ SRs, respectively. The signal shown in the figures and tables is the g2HDM signal with couplings ρ_{tt} =0.32, ρ_{tc} =0.05, and ρ_{tu} =0.85, and mass of 1000 GeV, which corresponds to the largest observed significance above the background only hypothesis.

Figure 9: Observed significance for a heavy scalar with a mass of 1000 GeV as a function of the three couplings normalised to the sum of the couplings. This normalisation is performed in order to eliminate one degree of freedom related to the total normalisation of the signal which is not relevant for the computation of the significance. The star indicates the coupling configuration leading to the highest observed significance of 2.81 standard deviations.

In general, good agreement between the data and fitted signal-plus-background yields is found across all event categories.

The systematic uncertainties with the largest impact on the signal strength originate from the modelling of *ttW* with and without additional heavy flavour jets, $t\bar{t}Z$, $t\bar{t}H$, and $t\bar{t}t\bar{t}$ processes. The search is dominated by statistical uncertainties.

Comparisons between data and the background prediction for the *DNN*SB distributions used in the different SRs is shown in Figures [11](#page-28-0) and [12.](#page-29-0) The binning used for the *DNN*SB distributions in the different SRs represents a compromise between preserving enough discrimination in the fit between the background and the signal for the different values of the heavy *H* mass considered and keeping the statistical uncertainty of the background prediction per bin well below 30%. The signal regions with the largest pre-fit tension between data and the background yields (shown in the blue dashed line) at high values of the *DNN*SB are the $2\ell SS$ ++ CAT tttq, the $2\ell SS$ ++ CAT tttt, the $2\ell SS$ ++ CAT sstt, and the $2\ell SS$ ++ CAT ttq regions. Within this model, the $\hat{\lambda}_{t\bar{t}W}$ remains higher than 1, as observed by other analyses. However, charge-asymmetric tensions both at low and high jet and h ist multiplicities are accommodated by the best fit g?HDM signal tensions both at low and high jet and *b*-jet multiplicities are accommodated by the best fit g2HDM signal, where the largest signal contributions in the $2\ell SS + CAT$ tttq and the $2\ell SS + CAT$ tttt regions originate mainly from ttq and ttt processes (excess at high jet multiplicities), and the largest signal contributions in the $2\ell SS$ ++ CAT sstt and the $2\ell SS$ ++ CAT ttq regions originate mainly from the corresponding targeted signals sstt and ttq processes (excess at low jet multiplicities).

Exclusion limits on the heavy Higgs boson mass are set for different choices of the couplings, as shown in Figure [13.](#page-30-0) Masses of an additional scalar boson m_H between 200-630 (200-840) GeV with couplings $\rho_{tt} = 0.4$, $\rho_{tc} = 0.2$, and $\rho_{tu} = 0.2$ are observed (expected) to be excluded at 95% confidence level. Limits on the mass heavy Higgs boson mass are also set for a scenario without coupling to two top quarks, $\rho_{tt} = 0$,

Figure 10: Comparison between data and the background prediction for the event yields in (a) the 17 signal region categories and (b) the 10 control region categories. The expected signal for $m_H = 1000$ GeV and (ρ_{tt} =0.32, ρ_{tc} =0.05, and ρ_{tu} =0.85) as well as the background contributions are shown after the likelihood fit to data ("Post-Fit") under the signal-plus-background hypothesis. The total background prediction before the likelihood fit to data ("Pre-Fit") is shown as a dashed blue histogram in the upper panel. The ratio of the data to the total prediction is shown in the lower panel, separately for post-fit signal-plus-background (black points) and pre-fit background (dashed blue line). The size of the combined statistical and systematic uncertainty in the background prediction is indicated by the blue hatched band.

(b)

 $\overline{\mathcal{Z}\mathcal{E}}_{\mathcal{U}(\Theta)_{(M_{\mathbf{e}_\mathcal{X},\mathcal{T})}}}$

 $\overline{\mathcal{Z}\mathcal{E}}_{\mathcal{U}_{(\Theta_{\mathcal{U}_{\mathcal{M}_{\mathcal{C}\mathcal{X}}}}M_{\mathcal{C}\mathcal{X}})}}$

³*^ℓ*IntC

³*^ℓ*MatC

³*ℓ*VV

³*ℓ*ttZ

 $\overline{\mathcal{Z}\mathcal{E}}_{\mathit{tt}(\mu)_{(T,M_{\mathit{ex}})}}$

 Ω 0.5 1F 1.5 Data / Pred.

1

10

 $\overline{\mathcal{Z}\mathcal{E}}_{\mathcal{U}(\mu)_{(M_{\mathbf{e}_\mathcal{X},\mathcal{T})}}}$

 $\overline{\mathcal{Z}\mathcal{E}}_{\mathit{tt}(\mu)_{(M_{\mathsf{e}_x, M_{\mathsf{e}_x}})}}$

 $\overline{\mathcal{Z}\mathcal{E}}_{\mathcal{U}(\Theta)_{(\mathcal{T},M_{\mathbf{e}_{\chi}})}}$

 $\rho_{tc} = 0.2$, $\rho_{tu} = 0.2$, resulting on an observed (expected) limit of 200-350 (200-580) GeV on the heavy Higgs boson mass. No limits can be set on scenarios without off-diagonal couplings, leading only to four-top final states with a coupling set $\rho_{tt} = 1$, $\rho_{tc} = 0$, $\rho_{tu} = 0$. The sensitivity of the analysis on the four-top final state is similar to previous ATLAS analyses [\[37\]](#page-36-4). The excluded mass is also presented as a function of two couplings under different assumptions, as shown in Figure [14.](#page-31-0)

The search is also used to set limits on RPV SUSY models using the existing DNNs that were trained for the g2HDM model. Figures $15(a)$ and $15(b)$ show the exclusion limits obtained on the higgsino and wino models respectively. Higgsinos (winos) with masses up to 585 (670) GeV are excluded. Figure [16](#page-32-2) shows limits on the smuon-bino model. Smuon masses up to 460 GeV are excluded, with weaker exclusion limits for small mass splittings between the smuon and the LSP, or for LSP masses close to the top-quark threshold.

Table 7: Post-fit yields of the 2 ℓ SS positively-charged signal regions. The best-fit signal for $m_H = 1000$ GeV and (ρ_{tt} =0.32, ρ_{tc} =0.05, and ρ_{tu} =0.85) is shown for a μ = 1.8 ± 0.8.

	2ℓ SS ++ CAT sstt	2ℓ SS ++ CAT ttg	2ℓ SS ++ CAT ttt	2ℓ SS ++ CAT tttq	2ℓ SS ++ CAT tttt
Signal	8±4	$16 + 7$	3.8 ± 1.7	$23 + 10$	4.2 ± 1.9
$t\bar{t}t\bar{t}$	0.2 ± 0.1	0.4 ± 0.1	2.3 ± 0.5	4.6 ± 0.9	7.8 ± 1.4
$t\bar{t}W$	231 ± 19	139 ± 10	219 ± 16	$68 + 7$	15 ± 2
$t\bar{t}H$	$17 + 3$	15 ± 2	$37 + 5$	$14 + 3$	6.1 ± 1.4
$t\bar{t}(Z/\gamma))$	$43 + 5$	24 ± 3	$53 + 5$	$14 + 1$	5.5 ± 0.8
$t\bar{t}\gamma$ (low mass)	5.3 ± 3.0	4.0 ± 2.4	4.9 ± 2.8	1.3 ± 0.8	0.6 ± 0.4
VV	$22 + 7$	11 ± 4	5.2 ± 1.9	2.2 ± 0.9	0.2 ± 0.1
tZ	24 ± 1	9.3 ± 0.6	5.2 ± 0.4	0.7 ± 0.1	0.01 ± 0.01
Non-prompt ℓ	$45 + 17$	20 ± 7	$19 + 6$	4.2 ± 1.9	0.8 ± 0.7
Mat Conv	$19 + 5$	5.9 ± 1.6	7.2 ± 2.1	1.7 ± 0.7	0.9 ± 0.2
OMisID	7.4 ± 2.7	1.7 ± 0.6	1.4 ± 0.5	0.2 ± 0.1	0.02 ± 0.01
Other	5.8 ± 2.0	4.0 ± 1.3	8.0 ± 2.2	6.1 ± 1.9	2.4 ± 0.6
Total	428 ± 15	250 ± 9	$367 + 12$	141 ± 9	43 ± 3
Data	434	261	342	138	46

Table 8: Post-fit yields of the 2 ℓ negatively-charged signal regions. The best-fit signal for $m_H = 1000$ GeV and $(\rho_{tt} = 0.32, \rho_{tc} = 0.05, \text{ and } \rho_{tu} = 0.85)$ is shown for a $\mu = 1.8 \pm 0.8$.

	$3\ell +$ CAT tttt	$3\ell +$ + CAT ttt	$3\ell +$ CAT tttq	3ℓ -- CAT tttt	3ℓ -- CAT ttt	3ℓ -- CAT tttq	4ℓ
Signal	1.2 ± 0.5	1.6 ± 0.7	2.9 ± 1.3	0.2 ± 0.1	0.2 ± 0.1	0.4 ± 0.2	0.05 ± 0.02
$t\bar{t}t\bar{t}$	3.7 ± 0.7	0.8 ± 0.2	1.7 ± 0.3	3.7 ± 0.7	0.9 ± 0.2	1.7 ± 0.3	1.5 ± 0.9
$t\bar{t}W$	4.6 ± 0.6	$100 + 7$	$23 + 3$	2.7 ± 0.4	55 ± 4	$12 + 2$	0.5 ± 0.1
$t\bar{t}H$	4.8 ± 1.0	$23 + 3$	7.5 ± 1.5	4.8 ± 1.0	$23 + 3$	7.6 ± 1.4	10 ± 3
$t\bar{t}Z/\gamma*$	11 ± 1	55 ± 6	$13 + 2$	11 ± 1	56 ± 6	$13 + 2$	24 ± 3
$t\bar{t}\gamma$ (low mass)	0.2 ± 0.2	2.6 ± 1.5	0.7 ± 0.4	0 ± 0	3.2 ± 1.8	0.5 ± 0.3	0 ± 0
VV	0.5 ± 0.2	11 ± 4	2.4 ± 0.9	0.4 ± 0.2	7.9 ± 3.0	2.1 ± 0.6	3.6 ± 1.3
tZ	0.27 ± 0.02	13 ± 1	2.5 ± 0.2	0.11 ± 0.01	7.2 ± 0.4	1.2 ± 0.1	0 ± 0
Non-prompt ℓ	0 ± 0	11 ± 4	1.9 ± 0.8	0.2 ± 0.1	$12 + 6$	1.1 ± 0.6	2.1 ± 0.3
Mat Conv	0.2 ± 0.1	3.2 ± 1.1	0.5 ± 0.3	0.1 ± 0.1	8±5	0.04 ± 0.01	0 ± 0
Other	1.9 ± 0.5	7.4 ± 2.3	3.3 ± 1.0	1.8 ± 0.5	5.9 ± 2.0	3.3 ± 1.0	2.7 ± 0.9
Total	28 ± 2	229 ± 6	60 ± 3	25 ± 2	$180 + 7$	$43 + 2$	45 ± 3
Data	30	236	53	27	195	47	45

Table 9: Post-fit yields of the 3 ℓ and 4 ℓ signal regions. The best-fit signal for $m_H = 1000$ GeV and ($\rho_{tt} = 0.32$, $\rho_{t} = 0.05$ and $\rho_{t} = 0.85$) is shown for a $\mu = 1.8 \pm 0.8$ ρ_{tc} =0.05, and ρ_{tu} =0.85) is shown for a $\mu = 1.8 \pm 0.8$.

Figure 11: Comparison between data and prediction for the *DNN*^{SB} distribution used in different signal region categories of the 2 ℓ SS channel: (a) 2 ℓ SS −−CAT sstt, (b) 2 ℓ SS −−CAT ttq, (c) 2 ℓ SS −−CAT ttt, (d) 2 ℓ SS −−CAT tttq, (e) $2\ell SS$ −− CAT tttt, (f) $2\ell SS$ ++ CAT sstt, (g) $2\ell SS$ ++ CAT ttq, (h) $2\ell SS$ ++ CAT ttt, (i) $2\ell SS$ ++ CAT tttq, and (j) $2\ell SS$ ++ CAT tttt. The expected signal for $m_H = 1000$ GeV and (ρ_{tt} =0.32, ρ_{tc} =0.05, and ρ_{tu} =0.85) as well as the background contributions are shown after the likelihood fit to data ("Post-Fit") under the signal-plus-background hypothesis. The ratio of the data to the prediction ("Pred.") is shown in the lower panel, separately for post-fit signal-plus-background (black points) and pre-fit background (dashed blue line). The size of the combined statistical and systematic uncertainty in the signal-plus-background prediction is indicated by the blue hatched band. The last bin in each Figure contains the overflow.

Figure 12: Comparison between data and prediction for the *DNN*SB distribution used in different signal region categories of the 3 ℓ and 4 ℓ channels: (a) 3 ℓ –− CAT ttt, (b) 3 ℓ –− CAT tttq, (c) 3 ℓ –− CAT tttt, (d) 3 ℓ ++ CAT ttt, (e) 3ℓ ++ CAT tttq, (f) 3ℓ ++ CAT tttt, and (g) 4 ℓ . The expected signal for $m_H = 1000$ GeV and (ρ_{tt} =0.32, ρ_{tc} =0.05, and ρ_{tu} =0.85) as well as the background contributions are shown after the likelihood fit to data ("Post-Fit") under the signal-plus-background hypothesis. The ratio of the data to the prediction ("Pred.") is shown in the lower panel, separately for post-fit signal-plus-background (black points) and pre-fit background (dashed blue line). The size of the combined statistical and systematic uncertainty in the signal-plus-background prediction is indicated by the blue hatched band. The last bin in each Figure contains the overflow.

Figure 13: Observed and expected exclusion limits at 95% confidence level on the heavy Higgs boson mass for the g2HDM signal model for different couplings choices: (a) $\rho_{tt} = 0$, $\rho_{tc} = 0.2$, $\rho_{tu} = 0.2$, (b) $\rho_{tt} = 0.4$, $\rho_{tc} = 0.2$, $\rho_{tu} = 0.2$, and (c) $\rho_{tt} = 1$, $\rho_{tc} = 0$, $\rho_{tu} = 0$. The yellow and green contours of the band around the expected limit are the $\pm 1\sigma$ and $\pm 2\sigma$ variations including all uncertainties, respectively. The theoretical prediction for the signal production cross section is also shown as a red line. The production cross section is the sum of the five production modes considered in the search.

Figure 14: Observed (solid line) and expected (dashed line) exclusion limits on the scalar mass as a function of the coupling under different assumptions: (a) $\rho_{tc} = \rho_{tu}$, (b) $\rho_{tu} = 0$, (c) $\rho_{tc} = 0$, and (d) $\rho_{tt} = 0$.

Figure 15: Expected and observed exclusion limits on the cross section × branching ratio of electroweakino production in RPV SUSY models as a function of the sparticle masses: (a) higgsino model, and (b) wino model. The yellow and green contours of the band around the expected limit are the $\pm 1\sigma$ and $\pm 2\sigma$ variations including all uncertainties, respectively. The theoretical prediction for the signal production cross section is also shown as a red line.

Figure 16: Expected and observed exclusion limits on the smuon plus bino RPV SUSY model. The yellow and green contours of the band around the expected limit are the $\pm 1\sigma$ and $\pm 2\sigma$ variations including all uncertainties, respectively. The diagonal grey lines indicates the allowed kinematic limit for the decays. The neutralino is assumed to decay to *tbl* or *bb*ν with equal probability.

9 Conclusion

A search for a general two Higgs doublet model is presented, where the heavy Higgs bosons feature flavour changing couplings. Such couplings allow for same-sign top and three-top production among others, with a sizeable charge asymmetry. The targeted final state is characterised by multiple leptons and multiple *b*-jets. In order to improve the sensitivity of the search, events are categorised according to the lepton multiplicity, total lepton charge, and a multi-output deep neural network classifier. The dominant backgrounds originate from $t\bar{t}W$, $t\bar{t}Z$, and $t\bar{t}$, and are estimated from Monte-Carlo simulation and normalised to data. The analysis if $\frac{1}{w}$, $\frac{1}{z}$, and $\frac{1}{w}$, and are estimated from Monte-Carlo simulation and normalised to data. The analysis is performed with proton-proton collision data at $\sqrt{s} = 13$ TeV collected from 2015 to 2018 with detector at the LHC, corresponding to an integrated luminosity of 139 fb−¹ . This search is the first collider result on general two Higgs doublet model with flavour violation. It also represents the first search to target explicitly beyond-the-standard-model production of three top quarks.

A mild excess is observed over the Standard Model expectation corresponding to a local significance of 2.81standard deviations for a signal with $m_H = 1000$ GeV and (ρ_{tt} =0.32, ρ_{tc} =0.05, and ρ_{tu} =0.85). The observed charge-asymmetric tensions both at low and high jet and *b*-jet multiplicities are accommodated by the best fit g2HDM signal, where the largest signal contributions in the $2\ell SS$ ++ CAT tttq and the 2ℓ SS ++ CAT tttt regions originate mainly from ttq and ttt processes (excess at high jet multiplicities), and the largest signal contributions in the $2\ell SS$ ++ CAT sstt and the $2\ell SS$ ++ CAT ttq regions originate mainly from the corresponding targeted signals sstt and ttq processes (excess at low jet multiplicities). Since the excess is not significant, 95% exclusion limits are also set on the mass and couplings of the heavy Higgs bosons. An additional scalar boson with couplings $\rho_{tt} = 0.4$, $\rho_{tc} = 0.2$, and $\rho_{tu} = 0.2$ is observed (expected) to be excluded at 95% confidence level for masses m_H between 200-630 (200-840) GeV. Additional mass limits are set for different coupling choices. For a fixed mass of $m_H = 400$ GeV exclusion limits are set on the allowed coupling strengths, as low as $\rho_{tt} = 0.3$, $\rho_{tc} = \rho_{tu} = 0.16$. Different assumptions are tested to set 2-dimensional exclusion limits on the three couplings. Additional models based on R-parity-violating supersymmetry with the lepton-number-violating coupling λ'_{i33} (with $i \in 2, 3$), are used to further interpret the results of the search. Scenarios with direct electroweak production of are used to further interpret the results of the search. Scenarios with direct electroweak production of higgsinos (winos) are excluded for masses between 200-585 (200-670) GeV. Smuons with masses between 225 and 600 GeVare excluded in a model with direct smuon production, decaying to a bino-like neutralino, which in turn decays via the λ'_{i33} coupling.

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