

Search for Flavor-Changing Neutral Current Interactions of the Top Quark and Higgs Boson in Final States with Two Photons in Proton-Proton Collisions at $\sqrt{s} = 13$ TeV

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Proton-proton interactions resulting in final states with two photons are studied in a search for the signature of flavor-changing neutral current interactions of top quarks (t) and Higgs bosons (H). The analysis is based on data collected at a center-of-mass energy of 13 TeV with the CMS detector at the LHC, corresponding to an integrated luminosity of 137 fb^{-1} . No significant excess above the background prediction is observed. Upper limits on the branching fractions (\mathcal{B}) of the top quark decaying to a Higgs boson and an up (u) or charm (c) quark are derived through a binned fit to the diphoton invariant mass spectrum. The observed (expected) 95% confidence level upper limits are found to be 0.019% (0.031%) for $\mathcal{B}(t \rightarrow Hu)$ and 0.073% (0.051%) for $\mathcal{B}(t \rightarrow Hc)$. These are the strictest upper limits yet determined.

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Flavor-changing quark decays mediated by neutral currents (FCNCs) are forbidden at tree level in the standard model (SM). They may proceed at higher orders in the perturbative expansion; however, these rates are heavily suppressed by the Glashow-Iliopoulos-Maiani mechanism [1] or Cabibbo-Kobayashi-Maskawa unitarity constraints [2]. The SM branching fractions for the decay of a top quark (t) into a Higgs boson (H) and up quark (u), $t \rightarrow Hu$, or charm quark (c), $t \rightarrow Hc$, are expected to be $\mathcal{O}(10^{-17})$ and $\mathcal{O}(10^{-15})$, respectively [3–6], well below the current sensitivity of the LHC experiments [7]. Thus, any observation of a $t \rightarrow Hq$ FCNC interaction would be an unambiguous sign of new physics. Here, the symbol q denotes either an up or charm quark.

In many scenarios of physics beyond the SM, the $t \rightarrow Hq$ branching fractions are enhanced by many orders of magnitude beyond the SM values. Notable beyond-the-SM models leading to enhanced FCNC interactions include those of warped extra dimensions [8], composite Higgs boson models [9], two-Higgs doublet models (2HDM) [10–13], including supersymmetric models with R -parity violation [14], and quark-singlet models [15]. While these scenarios lead to sizable FCNC interactions for a variety of neutral mediators other than the Higgs boson, including the Z boson, photon, and gluon, some of the most significant enhancements are found for $t \rightarrow Hq$ interactions. The $t \rightarrow Hc$ interaction in particular can be enhanced in 2HDM

models [16], including scenarios of flavor-violating Yukawa couplings [17] or 2HDM for the top quark [18–20].

Recent searches for FCNC interactions of the top quark and Higgs boson were performed by the ATLAS [7,21,22] and CMS [23] Collaborations, with Ref. [7] providing the strictest experimental upper limits on the $t \rightarrow Hu$ and $t \rightarrow Hc$ branching fractions at 0.12% and 0.11%, respectively. This Letter reports improved upper limits on these two branching fractions, exploiting both the associated production of a single top quark with a Higgs boson via an up or charm quark (ST production mode) and the decay of a top quark to a Higgs boson and an up or charm quark in $t\bar{t}$ production (TT production mode), as shown in Fig. 1, where the $H \rightarrow \gamma\gamma$ decay is considered.

The results are based on the analysis of proton-proton (pp) collisions at a center-of-mass energy of 13 TeV, targeting the $H \rightarrow \gamma\gamma$ decay mode. The data were collected with the CMS detector at the LHC between 2016 and 2018, and correspond to an integrated luminosity of 137 fb^{-1} .

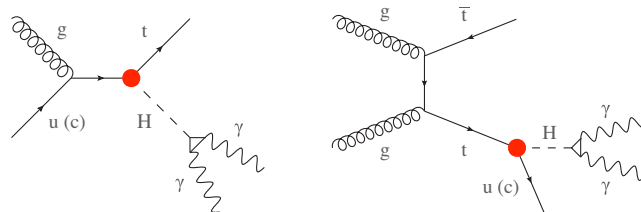


FIG. 1. Representative Feynman diagrams for the production modes considered: FCNC associated production of a single top quark with a Higgs boson (ST, left), and $t\bar{t}$ production with the FCNC decay of the top quark to a Higgs boson and an up or charm quark (TT, right). The Higgs boson decay to two photons is considered. The FCNC vertex in each process is denoted with a red circle.

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Tabulated results are provided in the HEPData record for this analysis [24].

The central feature of the CMS apparatus is a superconducting solenoid of 6 m internal diameter, providing a magnetic field of 3.8 T. Within the solenoid volume are a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter, each composed of a barrel and two end-cap sections. Forward calorimeters extend the pseudorapidity (η) coverage provided by the barrel and end-cap detectors. Muons are measured in gaseous detectors embedded in the steel flux-return yoke outside the solenoid. A more detailed description of the CMS detector, together with a definition of the coordinate system used and the relevant kinematic variables, can be found in Ref. [25].

The signal and background processes are simulated using several Monte Carlo (MC) programs. The signal samples corresponding to ST and TT production modes are simulated at leading order (LO) with MADGRAPH 5_aMC@NLO 2.4.2 (ST) and 2.6.0 (TT) [26]. Both the signal and background samples are interfaced with PYTHIA8.205 [27] for parton showering, fragmentation, and hadronization. The underlying event is also modeled with PYTHIA, with the CUETP8M1 [28] and CP5 [29] tunes used for the simulation of 2016 and 2017–2018 data, respectively. The parton distribution functions are taken from the NNPDF3.0 [30] set for simulation of 2016 data and the NNPDF3.1 [31] set for simulation of 2017–2018 data.

The FCNC interactions, including those with the Higgs boson as a mediator, can be described within the effective field theory framework in terms of dimension-six operators added to the SM Lagrangian [32,33]. The coefficients of these operators are best constrained by combining the results of the FCNC processes in which the Higgs boson, Z boson, photon, and gluon are the FCNC mediators. To perform this combination, it is important to have the most sensitive analysis for each individual process. In this Letter, the theoretical interpretation of the FCNC interactions with the Higgs boson as the mediator is done by using the following effective Lagrangian, which is equivalent to the effective field theory approach at LO,

$$\mathcal{L} = \sum_{q=u,c} \frac{g}{\sqrt{2}} \bar{t} \kappa_{Hqt} (F_{Hq}^L P_L + F_{Hq}^R P_R) q H + \text{H.c.}, \quad (1)$$

where g is the weak coupling constant, P_L and P_R are chirality projectors in spin space, κ_{Hqt} is the effective coupling constant, with $q = u$ or c , and F_{Hq}^L and F_{Hq}^R are left- and right-handed complex chiral parameters satisfying a unitarity constraint $|F_{Hq}^L|^2 + |F_{Hq}^R|^2 = 1$. The effective Lagrangian is implemented in the FEYNRULES package [34], with the universal FEYNRULES output [35] used to generate the model. The complex chiral parameters are set to $F_{Hq}^L = 1$ and $F_{Hq}^R = 0$. Up to two additional partons are generated at matrix element level for the TT production

mode. No additional partons are considered for the ST production mode to avoid overlap between the ST and TT modes. The hard-process simulation is interfaced with parton shower modeling using the MLM [36] matching prescription. Signal samples are generated in two scenarios, assuming exactly one nonzero coupling of unity: κ_{Hut} or $\kappa_{Hct} = 1$. The cross section of the ST production mode is calculated with MADGRAPH at LO precision and equals 72.6(10.0) pb for the scenarios of $\kappa_{Hut}(\kappa_{Hct}) = 1$. The $t\bar{t}$ cross section is taken as 832 pb, from calculation with the TOP++ program [37] at next-to-next-to-LO (NNLO) in perturbative quantum chromodynamics (QCD), which includes soft-gluon resummation to next-to-next-to-leading-logarithmic order. The cross section times branching fraction for the TT FCNC production mode depends on the branching fraction of $t \rightarrow Hu$ and $t \rightarrow Hc$, which is 0.144 (as calculated by MADGRAPH at LO) when assuming a coupling of $\kappa_{Hut} = \kappa_{Hct} = 1$. The effective coupling constant and branching fraction are related by

$$\kappa_{Hqt}^2 = \mathcal{B}(t \rightarrow Hq) \frac{\Gamma_t}{\Gamma_{Hqt}}, \quad (2)$$

where Γ_t is the full width of the top quark [38], and Γ_{Hqt} is the partial width of the anomalous $t \rightarrow Hq$ decay.

Calculations of the top quark transverse momentum (p_T) distribution at LO and next-to-LO (NLO) are known to show disagreement with the observed spectrum [39–42]. Since the effect may be partially due to missing higher-order calculations, the simulated top p_T distribution in TT signal events is corrected at generator level to match the NNLO QCD + NLO electroweak prediction [41].

Background processes with a Higgs boson decaying to two photons (resonant backgrounds), including ggH , vector boson fusion (VBF), WH , ZH , tHq , tHW , $t\bar{t}H$, and $b\bar{b}H$ production, are modeled with MADGRAPH 5_aMC@NLO2.4.2 at NLO [26] in QCD, with cross sections and decay branching fractions taken from Ref. [43]. Additional samples for SM Higgs boson processes are generated with POWHEG2.0 [44–47] at NLO in QCD. They are used to increase the size of the SM data sample needed for training the multivariate discriminants described below.

The MADGRAPH 5_aMC@NLO program is also used to simulate most background processes without a Higgs boson (nonresonant backgrounds). These include $t\bar{t} + \gamma\gamma$, $t\bar{t} + \gamma$, $t\bar{t} + \text{jets}$, $\gamma + \text{jets}$, $V + \gamma$, Drell–Yan, diboson, and $t + V$ production, where V is a W or Z boson. The diphoton background ($\gamma\gamma + \text{jets}$) is simulated with SHERPA2.2.4 [48], which includes tree-level processes with up to three additional jets, as well as box processes at LO accuracy. Simulation of nonresonant background samples is used for developing and optimizing the analysis, but this background is estimated from data in the fits used to extract a possible signal contribution. Finally, for both signal and

background samples, the detector response is modeled with the GEANT4 package [49].

The CMS trigger [50] selects events with two photon candidates satisfying a loose calorimetric identification [51], and asymmetric photon p_T thresholds of 30 and 18 (22) GeV for the data collected during 2016 (2017–2018). The trigger efficiency is $>95\%$ and is measured with the “tag-and-probe” method [52].

The particle-flow (PF) algorithm [53] reconstructs individual particles (photons, charged and neutral hadrons, muons, and electrons) by combining information from all subdetectors. Jets are built from PF particles using the anti- k_T algorithm [54,55] with a distance parameter of 0.4. The missing transverse momentum (\vec{p}_T^{miss}) [56] is defined as the negative vector p_T sum of all PF particles. Its magnitude is referred to as p_T^{miss} . The primary pp interaction vertex is taken as the vertex with the largest value of summed physics object p_T^2 . Charged hadrons originating from other pp interactions in the same or nearby bunch crossings are removed from the analysis. Jets from the hadronization of bottom quarks (b jets) are tagged by an algorithm based on the score from a deep neural network [57] called DEEPIET [58,59].

Higgs boson candidates are built from pairs of photon candidates. Photon candidates are reconstructed from energy clusters in the ECAL not linked to charged particle tracks (with the exception of converted photons). The photon energy is corrected for the containment of electromagnetic showers in the clustered crystals and the energy losses of converted photons with a multivariate regression technique based on simulation [51]. The ECAL energy scale in data is corrected based on studies of $Z \rightarrow e^+e^-$ events. The offline diphoton selection criteria are similar to, but more stringent than, those used in the trigger [51].

Photons are further required to satisfy a loose identification (photon ID [51]) criterion based on a boosted decision tree (BDT) classifier trained to separate photons from jets. In simulation, inputs to the photon ID such as shower shape and isolation variables are corrected with a chained quantile regression method [60] based on studies of $Z \rightarrow e^+e^-$ events. The cumulative distribution function of each variable in simulation is corrected with a set of BDTs that take the previously corrected features as inputs. This method ensures that both the individual distributions and correlations between variables in the MC simulation are corrected to match those in data.

After the selection described above, the diphoton invariant mass ($m_{\gamma\gamma}$) is required to be in the range 100–180 GeV. The upper bound of 180 GeV is selected to ensure a sufficient number of events for the procedures used to model the nonresonant background and to validate the modeling of input features to the BDTs, both described later. We additionally impose mass-dependent photon p_T requirements of $p_T/m_{\gamma\gamma} > 1/3$ and $> 1/4$ for the highest p_T (leading) and second-highest p_T (subleading) photons,

respectively. Events are next divided into two mutually exclusive channels. The leptonic channel preselection is aimed at selecting events with a leptonically decaying top quark, and requires the presence of ≥ 1 jet with $p_T > 25$ GeV and $|\eta| < 2.4$, ≥ 1 isolated lepton (e or μ) with $|\eta| < 2.4$, and $p_T > 10(20)$ GeV for electrons (muons) [61]. The hadronic channel preselection targets events with a hadronically decaying top quark, requiring at least three jets, of which at least one is identified as a b jet, and no isolated leptons (e/μ).

Dedicated BDT discriminants are employed in each channel to distinguish signal (ST and TT production modes) from background events. Separate BDTs are trained for each of the two nonzero κ_{Hqt} coupling scenarios, each of the two channels, and each of the two primary categories of SM background, resonant (BDT-res) and nonresonant (BDT-nonres). This results in eight BDTs in total: one for each coupling (κ_{Hut} or κ_{Hct}), channel (hadronic or leptonic), and background (resonant or nonresonant). The BDTs are trained with the XGBOOST [62] framework on MC samples of signal and background processes, with one exception as noted below. The nonresonant background MC samples include $\gamma + \text{jets}$, $\gamma\gamma + \text{jets}$, $t\bar{t} + \text{jets}$, $t\bar{t} + \gamma$, $t\bar{t} + \gamma\gamma$, and $V + \gamma$ processes, as well as a variety of other rarer backgrounds (designated in figures as “Other”), including $t\bar{t}Z$, $t\bar{t}W$, WW , WZ , ZZ , and $t + \gamma + \text{jets}$. The resonant background MC samples include $t\bar{t}H$, WH , ZH , VBF, ggH , tHq , and tHW . In the training, all backgrounds are normalized to their SM cross sections.

The dominant backgrounds after the hadronic channel preselection are the multijet and $\gamma + \text{jets}$ processes, where at least one jet is misidentified as a photon. To improve the description of these backgrounds for training the machine learning algorithms, they are modeled using a sample of data events in which one photon candidate fails the photon ID requirement, following the procedure of Ref. [63]. For this procedure, the photon ID value of the photon candidate failing the photon ID requirement is replaced by a value drawn from the MC photon ID distribution for misidentified jets passing the photon ID requirement. This sample of events from data, denoted with $(\gamma) + \text{jets}$, is used instead of the simulated $\gamma + \text{jets}$ sample in the hadronic nonresonant background BDT training.

Input features of both BDT-res and BDT-nonres include the kinematic properties of the physics objects: jets, leptons, photons and diphotons (excluding $m_{\gamma\gamma}$), jet and lepton multiplicities, p_T^{miss} , b tagging scores of jets from the DEEPIET algorithm, and the output of the photon ID BDT for both photons. The p_T of the individual photons and diphotons are normalized by $m_{\gamma\gamma}$ to ensure the inputs to the BDTs cannot be used to calculate $m_{\gamma\gamma}$. The output of a variety of algorithms aimed at reconstructing top quarks in each event are also used as input features to the BDTs, as detailed below.

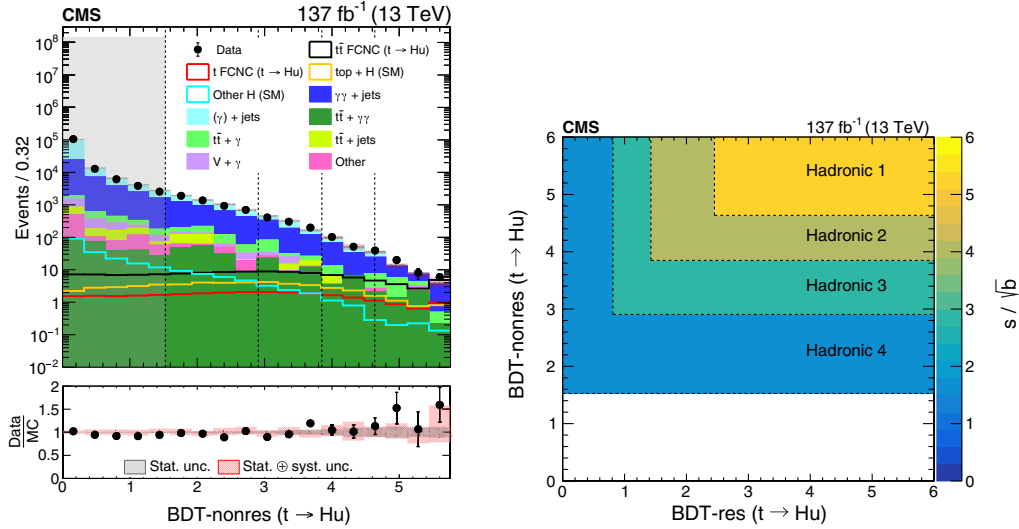


FIG. 2. Left: distribution of the BDT-nonres scores used for the hadronic event categorization targeting $t \rightarrow Hu$ FCNC interactions from data (points) and predictions from simulation (colored histograms). The “Other” category includes contributions from $t\bar{t}Z$, $t\bar{t}W$, WW , WZ , ZZ , and $t + \gamma + \text{jets}$. The “top + H” category includes $t\bar{t}H$, tHq , and tHW , while the “Other H” category includes ggH , VBF , WH , and ZH . The nonresonant background histograms are stacked, while the two signal, “Other H”, and “top + H” distributions are shown separately. Boundaries defining event categories are indicated with dotted lines in the upper panel. Events in the gray shaded region are not considered in the analysis. The lower panel shows the ratio of the data to the sum of the nonresonant background predictions. The simulated signal and background distributions are normalized to the integrated luminosity of the data, assuming a coupling of unity for the signal. Statistical and total (statistical \oplus systematic) background uncertainties are represented by the gray- and red-shaded bands, respectively. The $(\gamma) + \text{jets}$ sample of multijet and $\gamma + \text{jets}$ events from data is not assigned a systematic uncertainty, as described in the text. Right: hadronic event categorization targeting $t \rightarrow Hu$ FCNC interactions from requirements placed on BDT-nonres (horizontal dotted lines) and BDT-res (vertical dotted lines). The color denotes the s/\sqrt{b} of each category.

First, a set of mass variables is used for events with at least four jets in the hadronic channel. The invariant mass of the diphoton candidate plus the light jet from $t \rightarrow Hq$ decays ($m_{\gamma\gamma j}$) should be consistent with the top quark mass (m_t), as should the invariant mass of the three jets (m_{jjj}) from the hadronically decaying top quark candidate. The mass variables $m_{\gamma\gamma j}$ and m_{jjj} are constructed from three of the leading four jets by choosing the combination that minimizes the quantity $\Delta M = |m_{\gamma\gamma j} - m_t| + |m_{\text{jjj}} - m_t|$. Second, kinematic reconstructions of top quarks and their decay products for both hadronic and leptonic decays are performed, with the reconstruction for hadronic decays similar to that in Ref. [23] and the reconstruction for leptonic decays similar to that in Ref. [64]. The kinematic properties of the reconstructed top quarks and their decay products are used as input features to the BDTs. Third, a set of neural networks is trained with the TMVA package [65] on MC samples of signal processes to identify the jets and leptons that originate from the top quark(s) decays. Permutations of jets and leptons matched to a top quark decay are considered as signal, while all incorrect permutations are considered as background. Separate neural networks are trained for each signal production mode (ST and TT) and each channel (hadronic and leptonic).

The modeling of the input features is validated by comparing their distributions in data and simulation for

events passing the preselection and having $m_{\gamma\gamma}$ in the sidebands, defined as the $m_{\gamma\gamma}$ ranges of 100–120 or 130–180 GeV. The resulting BDT scores are also validated in the same way, as shown in Fig. 2 for the $t \rightarrow Hu$ search. We note that the sample of events from data used to model the multijet and $\gamma + \text{jets}$ processes is only used in the BDT training and optimization and does not enter the fits used to extract possible FCNC signals. Consequently, no systematic uncertainty is considered for the sample, despite that is not a perfect representation of these processes.

For each scenario of a nonzero FCNC coupling (κ_{Hut} or $\kappa_{Hct} = 1$), and for each channel (hadronic or leptonic), events are either removed from consideration or assigned to categories. The categories are defined by ranges of the BDT-nonres and BDT-res scores, shown, for example, with the four categories in the $t \rightarrow Hu$ search in the hadronic channel indicated by the horizontal and vertical dotted lines in Fig. 2 (right). In the same fashion, three categories are defined for the $t \rightarrow Hu$ search in the leptonic channel, using the leptonic BDT-nonres and BDT-res scores. The procedure is repeated for the $t \rightarrow Hc$ search, resulting in a total of seven categories for each of the $t \rightarrow Hu$ and $t \rightarrow Hc$ searches. Each resulting set of seven $m_{\gamma\gamma}$ distributions is then fitted simultaneously to extract a possible FCNC signal. The categories for the $t \rightarrow Hu$ ($t \rightarrow Hc$)

search contain between 13%–26% (2%–5%) of the total signal from ST production.

The expected $m_{\gamma\gamma}$ distributions of signal and resonant background events are modeled using the sum of a double-sided Crystal Ball function [66] and a Gaussian function. The models are derived from simulation for signal as well as each type of resonant background (ggH , VBF, WH , ZH , tHq , tHW , $t\bar{t}H$, and $b\bar{b}H$), with the Higgs boson mass (m_H) fixed to its most precisely measured value of 125.38 GeV [67]. The nonresonant background is modeled directly from data, using the discrete profiling method [68], in which the systematic uncertainty associated with the choice of analytic function used to model the $m_{\gamma\gamma}$ distribution is treated as a discrete nuisance parameter. All sources of experimental and theoretical systematic uncertainties are treated as nuisance parameters.

The total $t\bar{t}$ cross section uncertainty is taken as 6%, estimated from the uncertainty in the $t\bar{t}$ NNLO cross section, due to variation of the factorization (μ_F) and renormalization (μ_R) scales, the parton distribution functions, and strong coupling constant α_s [69–72]. We assign an uncertainty in the ST signal production mode cross section of 30% that is typically attributed to the missing higher-order corrections in the LO generation used in the analysis. The typical effect of varying μ_F and μ_R on the shapes of the BDT-nonres and BDT-res distributions is around 1% (10%) for the TT(ST) signal production mode. The uncertainties in the cross sections of the resonant background processes are estimated by varying μ_F and μ_R , PDFs, and α_s [43].

The dominant experimental uncertainties are those related to the b jet and photon identifications, the integrated luminosity [73–75], the jet energy scale and resolution, reconstruction of \vec{p}_T^{miss} , and the preselection and trigger efficiencies. The impact of each of these uncertainties on the final upper limits is $\leq 5\%$.

No significant excess above the background prediction is observed in any of the categories. Binned fits of the $m_{\gamma\gamma}$ distributions are performed simultaneously in each set of seven categories (14 total) to extract the 95% confidence level (CL) upper limits on $\mathcal{B}(t \rightarrow Hu)$ and $\mathcal{B}(t \rightarrow Hc)$. The derivation of upper limits assumes one nonzero coupling at a time and uses the modified frequentist approach for confidence levels (CL_s technique), with the LHC profile likelihood ratio as a test statistic [76,77] in the asymptotic approximation [78].

The $m_{\gamma\gamma}$ distributions for events entering the analysis are shown in Fig. 3, with events weighted by the quantity $S/(S+B)$ of their respective category. Here S (B) is defined as the number of signal (background) events in the range $m_H \pm \sigma_{\text{eff}}$, where σ_{eff} is the effective width of the signal model, defined as half of the range that contains 68% of the total number of events. The number of signal events S is normalized to the expected 95% CL upper limit on $\mathcal{B}(t \rightarrow Hq)$.

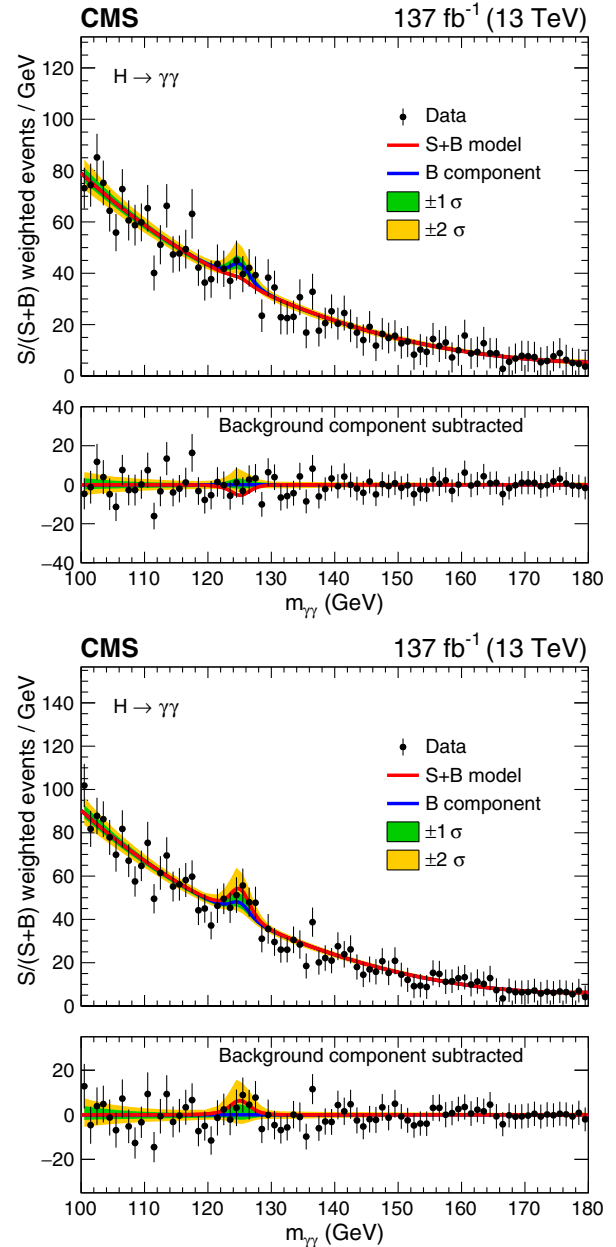


FIG. 3. The diphoton invariant mass distribution for the selected events from data (black points), and the results of the fits to the signal plus background models (solid red curve), and the background model alone (dotted blue curve), for the categories targeting $t \rightarrow Hu$ FCNC interactions (left) and $t \rightarrow Hc$ FCNC interactions (right). The signal model is normalized to the best-fit value. The green and yellow bands give the ± 1 and ± 2 standard deviation uncertainties in the background model (dotted blue curve). The background model includes $H \rightarrow \gamma\gamma$ events from SM processes. Events are weighted by the $S/(S+B)$ of their respective categories. The lower panels show the same information, but with the background component subtracted.

The observed and expected 95% CL upper limits are shown in Fig. 4 for $\mathcal{B}(t \rightarrow Hu)$ (upper) and $\mathcal{B}(t \rightarrow Hc)$ (lower), for each of the seven categories and combined. The observed (expected) 95% CL upper limits on $\mathcal{B}(t \rightarrow Hu)$

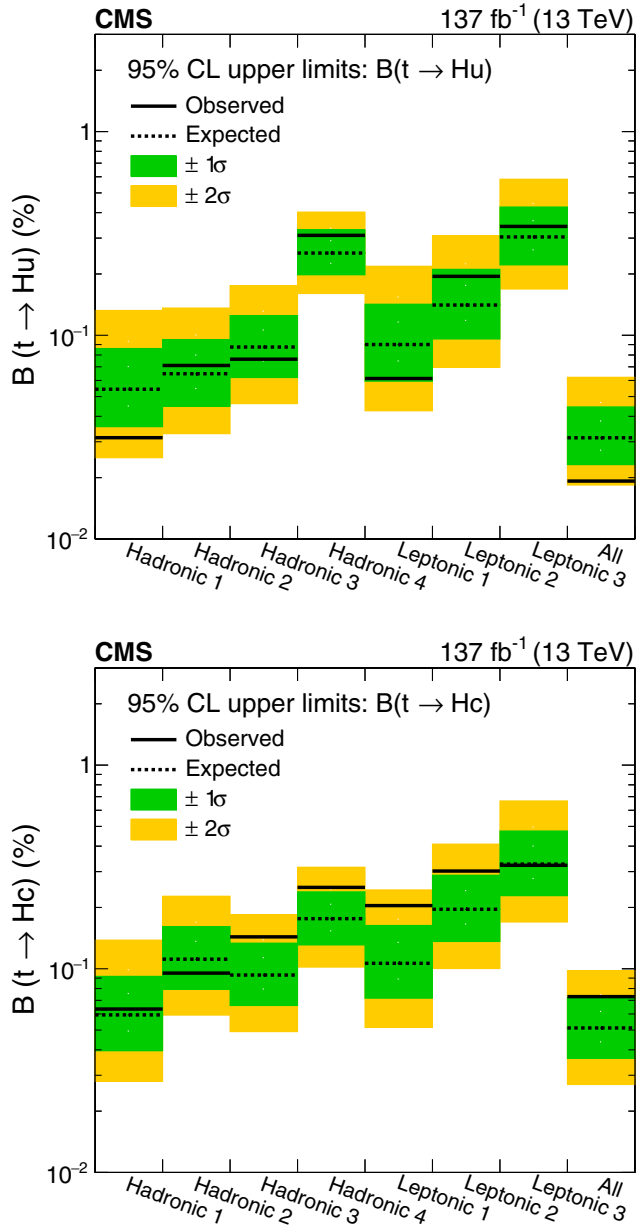


FIG. 4. The observed (solid line) and expected (dotted line) 95% CL upper limits on $\mathcal{B}(t \rightarrow Hu)$ (left) and $\mathcal{B}(t \rightarrow Hc)$ (right) for each of the hadronic and leptonic categories, defined as described in the text. The last bin gives the overall combined upper limit. The ± 1 and ± 2 standard deviation variations on the expected limit are given by the green and yellow bands, respectively.

and $\mathcal{B}(t \rightarrow Hc)$ are 0.019% (0.031%) and 0.073% (0.051%), respectively. The corresponding observed (expected) 95% CL upper limits on $|\kappa_{Hut}|$ and $|\kappa_{Hct}|$, derived with Eq. (2), are 0.037(0.047) and 0.071(0.060), respectively.

In summary, we have presented a search for flavor-changing neutral current interactions of the top quark (t) and Higgs boson (H) in proton-proton collisions at a

center-of-mass energy of 13 TeV. The processes considered include both the associated production of a single top quark with a Higgs boson via an up or charm quark, and the decay of a top quark to a Higgs boson and an up or charm quark in $t\bar{t}$ production. No significant excess above the background prediction is observed. The observed (expected) 95% CL upper limits on $\mathcal{B}(t \rightarrow Hu)$ and $\mathcal{B}(t \rightarrow Hc)$ of 0.019% (0.031%) and 0.073% (0.051%), respectively, are the most stringent experimental limits published to date.

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