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n-type doping in Cu_2O by halogen impurities: a first-principles study[1] QIONG BAI, MENG TAO, QIMING ZHANG, University of Texas at Arlington — The present work focuses on first-principles calculations on n- type doping by F, Cl, and Br impurities in Cu_2O under solution-grown environments. From the formation energy point of view, the substitution of oxygen in Cu_2O is favored over the interstitial sites. The electronic structures after doping are carefully studied.

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