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First-principles DFT+GW study of oxygen doped CdTe[1] WALTER ORELLANA, Departamento de Ciencias Físicas, Universidad Andres Bello, MAURICIO A. FLORES, Departamento de Física and Departamento de Matemáticas, Facultad de Ciencias, Universidad de Chile, EDUARDO MENÉNDEZ-PROUPIN, Departamento de Física, Facultad de Ciencias, Universidad de Chile — The role of oxygen doping in CdTe is addressed by first-principles calculations. Formation energies, charge transition levels and quasiparticle defect states are calculated within the DFT+GW formalism. The formation of a new defect is identified, the ($O_{Te} - Te_{Cd}$) complex. This complex is energetically favored over both isovalent (O_{Te}) and interstitial oxygen (O_i). We find that incorporation of oxygen passivates the harmful deep energy levels derived from Te antisites, suggesting an improvement in the efficiency of CdTe based solar cells. Our calculations indicate that both (O_{Te}) and (O_i) have low formation energies. Moreover, (O_{Cd}) is only stable in the neutral charge state and undergoes a Jahn-Teller distortion. The (V_{Cd}−O_{Te}) complex is found to be a shallow acceptor with a high formation energy. We also report an oxygen-related interstitial defect, which plays a key role in the diffusion mechanism of oxygen in CdTe.

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Eduardo Menéndez-Proupin
Departamento de Fsica, Facultad de Ciencias, Universidad de Chile

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