

Symmetry and thermodynamics of tellurium vacancies in cadmium telluride

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The equilibrium geometries and thermodynamic properties of anion vacancies in cadmium telluride, as predicted by density functional theory, are revisited using semilocal and hybrid density functionals. We find that stable configurations in different charge states can only be found after a systematic search considering several starting geometries. The stable charge states, 0 and 2+, display closed-shell electronic configurations, without deep bandgap levels. The 2+ charge state has a T_d symmetry with an outward relaxation, while the neutral state is a mixture of configurations with C_{2v} and C_{3v} symmetries, both with the same energy and a negligible energy barrier. Therefore, the neutral charge state presents an effective T_d symmetry. Configurations with different symmetries, e.g., D_{2d} , can exist as metastable states. We show that certain configurations may seem falsely stable due to several facts: the bandgap error of generalized gradient approximation, the k-point sampling used in small supercells, or the use of a restricted set of starting geometries. We believe that the HSE06 hybrid functional allows to obtain accurate formation energies and geometries. We analyze the effect of the spin-orbit coupling and GW quasiparticle corrections to the HSE06 results, and find no qualitative differences. The spin-orbit coupling and GW corrections to the HSE06 energies partially cancel each other. Finally, we investigate the divacancy $VCdVTe$. The obtained formation energies suggest that isolated tellurium vacancies in neutral charge state can be found only in Te-poor growth conditions, coexisting with divacancies.