Abstract Submitted
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Ab initio study of the effect of vacancies on the thermal conductivity NAKIB PROTIK, Boston College, JESUS CARRETE, NATALIO MINGO, LITEN, CEA-Grenoble, NEBIL KATCHO, CIC EnergiGUNE, DAVID BROIDO, Boston College — Point defects and vacancies in particular can have a profound impact on phonon thermal transport. Examples are seen in diamond [1] and cubic boron arsenide [2, 3] where large C and As vacancy concentrations give much lower thermal conductivity than expected [2, 3]. Here, we calculate the phonon-vacancy scattering rates using an *ab initio* Green's function approach [1], which treats the scattering to all orders in contrast to standard perturbation theory approaches. The lattice thermal conductivity, k, is calculated from first principles by solving the Boltzmann transport equation for phonons, with interatomic force constants determined using density functional theory. The reduction in k with vacancy defect density is assessed. The phonon-vacancy scattering can show significant differences using the Green's function method compared to what would be predicted from the perturbative Born approximation, consistent with previous findings for diamond [1].
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