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Application of Hybrid Functionals to Semiconductor Surfaces
MANISH JAIN, University of Texas, Austin and Department of Physics, University of California, Berkeley, JAMES CHELIKOWSKY, University of Texas, Austin, STEVEN LOUIE, Department of Physics, University of California, Berkeley and Lawrence Berkeley National Laboratory — Hybrid functionals within Generalized Kohn Sham formalism have been shown to give good band gaps for semiconductors and small band gap insulators, when a particular mixing of nonlocal exchange is included. We explore the use of hybrid functionals for semiconductor surfaces. Semiconductor surfaces often have multiple band gaps - the bulk-state gaps and surface-state gaps - which can be quite different. This study examines the applicability of hybrid functionals for such systems. In particular, we focus on diamond and silicon and their (100) and (111) surfaces, where surface states exist and are known to have lower band gaps. We employ the hybrid functionals - PBE0, HSE and B3LYP - to examine the structural and electronic properties of these surfaces.
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