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Equivalent parameters for empirical pseudopotential and k•p models

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After thirty-five years the empirical pseudopotential electronic band structures that were fitted by James R. Chelikowsky and Marvin L. Cohen (Phys. Rev. B 14, 556, 1976) are still used widely and are regarded by some workers as being among the best. Although the original paper by Chelikowsky and Cohen has received more than 600 citations, not all subsequent workers have been able to reproduce the band structures accurately. In a few of the citing papers, significant errors were introduced by, for example, incorrectly adding the effects of non-locality in the core potentials and spin-orbit coupling. In the original work both of these effects were added as perturbations. In the present work it is shown that the original calculations of Chelikowsky and Cohen can be reproduced accurately, even without the use of perturbation theory. This reproduction allows the original band structures to be used with great ease. As an example, the original band structures are used as input to an optimization calculation which produces equivalent fourteen-band and thirty-band (full-zone) k•p parameters for the original eleven diamond and zinc-blende semiconductors. The original band structures are also compared to those obtained through state-of-the-art ab-initio density functional calculations.

Level (Hons, MSc,
   PhD, other)?

MSc

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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