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A variational polaron-self-interaction corrected total-energy functional for charge excitations in wide-gap insulators[1] BABAK SADIGH, LLNL, PAUL ERHART, Chalmers University, Sweden, DANIEL ABERG, LLNL — A simple modification of the density-functional theory (DFT) total energy functional is proposed that corrects for the polaron self-interaction error in the semilocal approximations (LDA/GGA) to the exchange-correlation potential. It can accurately reproduce polaron formation in widegap insulating materials. Extensive study of the potential-energy landscapes of self-trapped holes in alkali halides is performed and agreeable comparison with hybrid-DFT and experiment is obtained. The new functional is general, simple to implement and its variational formulation allows for ab-initio molecular-dynamics simulations of polarons in widegap insulators regardless of complexity.

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