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First-principles Studies of ErAs and ErAs/GaAs Heterostructures KRIS T. DELANEY, NICOLA A. SPALDIN, CHRIS G. VAN DE WALLE, Materials Research Laboratory, UC Santa Barbara — We present a computational investigation of the materials properties of rare-earth pnictides. ErAs, a semimetal with rock-salt structure, has been demonstrated to grow epitaxially on GaAs substrates with a continuous As sublattice and low strain. Such structures have the potential to provide high-quality thermoelectric materials. Using plane-wave based density-functional methods we have performed a detailed investigation of the effects of f electrons on the electronic and atomic structure, using both norm- conserving pseudopotentials and the projector-augmented-wave method. Our preliminary results indicate that it is possible to obtain an adequate description of the band structure without having to include the f electrons as valence electrons. The resulting reduction in computational complexity allows us to perform explicit simulations of heterostructures. We have also calculated deformation potential constants, to be used in detailed comparisons with experiments where strain affects the band structure.

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