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Construction of a first-principles-based second-principle method containing electronic and lattice degrees of freedom PABLO GARCIA-FERNANDEZ, Departamento CITIMAC, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, 39005 Santander, Spain, JACEK WOJDEŁ, JORGE ÍÑIGUEZ, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, E-08193 Bellaterra, Spain, JAVIER JUNQUERA, Departamento CITIMAC, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, 39005 Santander, Spain — First principles simulations are limited in their application to small physical systems containing, in most realistic cases, a few hundred atoms. While not so restricted in size, second-principles simulations are usually focused on either electronic or lattice properties. However, both degrees of freedom are important in many physical problems and should be treated on the same footing. We present here an approach that accurately reproduces first-principles results for systems including reasonably localized electrons like transition-metal oxides or semiconductors. This scheme combines a reliable model potential for the lattice with a modified tight-binding method including both long-range electron-electron repulsions and short-range strong correlations. The interaction of lattice and electron degrees of freedom includes both electrostatics and short-range terms allowing the description of a wide range of phenomena. We illustrate the applicability of our method by tackling two difficult problems where the interaction between lattice and electrons is fundamental, such as the formation of polarons in bulk $SrTiO_3$ and the metallicity at the $LaAlO_3/SrTiO_3$ interface.

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