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Supercell issues in density functional calculations P.A. SCHULTZ, R.M. VAN GINHOVEN, T.R. MATTSSON, A.E. MATTSSON, Sandia National Laboratories — Simulations within density functional theory (DFT) are a common component of research into the physics of materials. With the broad success of DFT, it is easily forgotten that computational DFT methods invariably do not directly represent simulated properties, but require careful construction of models that are computable approximations to a physical property. Perhaps foremost among these computational considerations is the routine use of the supercell approximation to construct finite models to represent infinite systems. Pitfalls in using supercells (k-space sampling, boundary conditions, cell sizes) are often underappreciated. We present examples (e.g. vacancy defects) that exhibit a surprising or significant dependence on supercells, and describe workable solutions. We describe procedures needed to construct meaningful models for simulations of real material systems, focusing on k-space and cell size issues. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04- 94AL85000.

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