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Ab initio metal-insulator transition in doped silicon

The Anderson metal-insulator transition (MIT)has long been studied, but there is still no agreement on its critical exponent when comparing experiments and theory. In this work, we employ ab initio methods to study the MIT that occurs in sulfur-doped silicon (Si:S) when the concentration of the dopants is increased. We use linear-scaling DFT, as implemented in the ONETEP code, to study model Si:S systems at realistic concentrations (i.e. a few impurities, in a large simulation cell). We then use the resulting ab initio Hamiltonian to build an effective tight-binding Hamiltonian for larger systems close to the critical concentration of the MIT. We finally use multifractal finite-size scaling to characterise the MIT in Si:S, including the ab-initio-determined possible interactions between the donated electrons.