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Disorder effects in solid state systems beyond a single-site prospective: theories and applications ALBERTO MARMODORO, ARTHUR ERNST, Max-Planck-Institut für Mikrostrukturphysik, Halle — We review development and applications of improvement attempts upon the original Coherent Potential Approximation for the first-principles treatment of disordered systems. The single-site theory is examined in its basic aspects of analyticity and convergence, and compared with alternative methods for the study of solid state systems where a rigorous application of Bloch's theorem is no longer possible. The aspects of local environment effects, short-range ordering and off-diagonal disorder are considered in different extension proposals, in tight-binding and ab-initio illustrations based on multiple-scattering theory. In this context, results from application of a generalized version of the method are discussed evaluating some effects of disorder in solid state metallic solutions, molar doping materials for fuel cell technology, and magnetic compounds and excitations. Results from alternative methodologies such as supercell or special quasi-random structure approximations are also examined.

Alberto Marmodoro
Max-Planck-Institut für Mikrostrukturphysik, Halle

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