Electronic structure of randomly substituted solids using DFT methods

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Two distinct problems often arise when the first principle methods are used to study the electronic structure of real materials: 1) how to account for disorder and 2) how to present the results in a meaningful way. Often, the calculations are performed assuming periodic boundary conditions within so-call supercell approximation. It is also typical to choose the smallest cell size possible in order to reduce computational costs. Of course, the smallest cell has only one impurity or defect that combined with periodic boundary conditions can not account for random impurity distribution in real materials. Here we too use the supercell approximation but allow some degree of randomness in the impurity distribution across the super cell. We then use a simple procedure to present calculated band structures in a way as seen by ARPES (unfolding) and demonstrate the effect of impurity scattering on the electronic structure, Fermi surface and Lindhard function in transition metal substituted iron pnictides. We find that Ni, Cu and Zn strongly modify the band structure and the Fermi surfaces that very approximately looks like a chemical potential shift. The results clearly demonstrate that disorder destroys momentum as a good quantum number and gives rise to self energy that shows strong energy dependence.