Quantum-mechanical comparative study of ground states in Fe_3Al

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There is a long-lasting problem with quantum-mechanical calculations and their incorrect prediction of the ground-state structure of Fe_3Al. Many exchange-correlation functionals lead to the preference of the $L1_2$ structure instead of experimentally found $D0_3$ phase. Using the VASP code we calculated energy-volume curves for five exchange-correlation functionals combined with six different projector-augmented-wave potentials. The exchange-correlation functionals employed are Perdew-Wang 91 (PW91), Perdew-Burke-Ernzerhof (PBE), revised Perdew-Burke-Ernzerhof (rPBE), Armiento-Mattson (AM05), and Perdew-Burke-Ernzerhof revised for solids (PBEsol). The projector-augmented-wave potentials for Fe and Al are GGA (Fe), GGA with p semi-core states treated as valence states (Fepv), PBE potentials (PBE), PBE with p semi-core states treated as valence states (PBEpv), potentials used for GW calculations (GW) and GW with s and p semi-core states treated as valence states (GWsv). We used the energy preference of the $D0_3$ structure as the most important criterion: the energy difference $E(D0_3) - E(L1_2)$ was calculated and combinations that prefer $L1_2$ structure were not considered. Lattice parameter was the second criterion: combinations exhibiting a difference from the experimental value larger than 2% difference were rejected. Finally, we analyzed also the differences between the calculated and experimental bulk modulus. Considering the above mentioned criteria, we select the Perdew-Wang 91 exchange-correlation functional using Vosko-Wilk-Nusair interpolation for description of the ground state of Fe_3Al. Here the energy difference $E(D0_3) - E(L1_2)$ varies from -4.45 to -7.10 meV/atom, the difference between the calculated and experimental lattice constant lies between -0.85 and -1.01% and the calculated bulk modulus differs from the experimental one by values within the range from 22.7 to 23.6%.

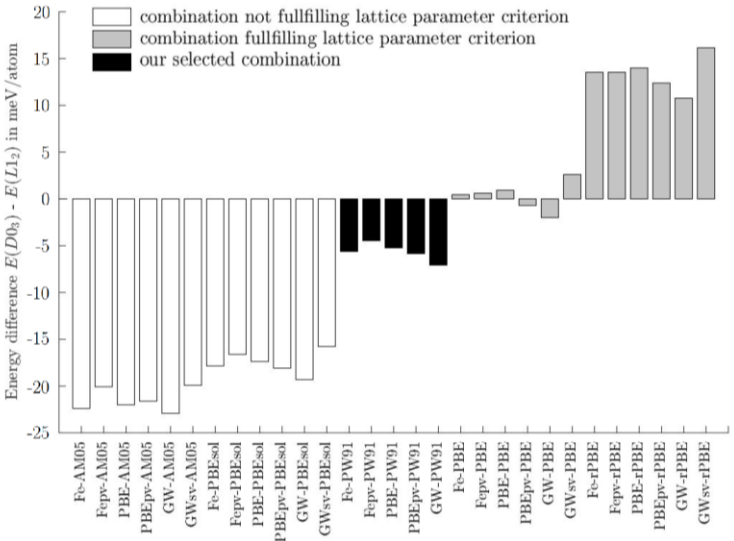

Figure 1 Energy difference of $E(D0_3)$–$E(L1_2)$ for different combinations of exchange-correlation functionals and projector-augmented-wave potentials in Fe_3Al calculation.