Dynamic correlation effect on small Fe-clusters

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We study the dynamic correlation effect on the magnetization of small isolated Fe and Ni clusters. The local Green's function is constructed by downfolding the Kohn-Sham states of VASP calculation with PAW potential, and the dynamic correlation effect is taken into account by the dynamical mean field theory with IPT solver. It's found that, for clusters of 10-20 Fe atoms, the dynamic correlation effect tends to decrease the magnetization.

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