Abstract Submitted
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Ab initio **calculations for the photoelectron spectra of iron clusters**[1] SHEN LI, Department of Physics and Astronomy, Rutgers the State University of New Jersey, Piscataway, NJ 08854,USA, MANUEL ALEMANY, Departamento de Física de la Materia Condensada,Facultad de Física, Universidad de Santiago de Compostela, E-15872, Spain, JAMES CHELIKOWSKY, Department of Physics and Chemical Engineering, Institute of Computational Engineering and Sciences, University of Texas, Austin, Texas 78712, USA — We studied negatively charged iron clusters Fe_n^- $(n = 3-6)$. We use a real-space pseudopotential approach based on the density-functional theory within local spin density approximation. The real space approach assumes no explicit basis. Wave functions are evaluated on a uniform grid; only one parameter, the grid spacing, is used to control the convergence of the electronic properties. Charged states are easily handled in real space, in contrast to method based on supercells where electrostatic divergences require special handling. For each cluster, we determined the ground state structure. To compare with the experimental photoelectron spectra, we calculated the electron binding energies, which include the final state relaxation effects. Our results for the photoelectron spectra, are able to reproduce the main features of the experiments. Our results for the magnetic moment of each cluster agree well with the other theories.

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