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Structural and Magnetic Properties of Iron Clusters

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Introduction

Electronic, magnetic, and chemical properties of Fe nanoparticles are of particular interest for materials science, engineering, and metallurgical applications, including biomedical applications (e.g., medical imaging, cancer treatment, etc.). In this study, we search for the most stable geometries of the Fe clusters, Feₙ, up to n=8. Binding energies, magnetic moments, bond lengths, bond angles, and charge densities of clusters are computed and compared to the available experimental data. The various cluster isomers were examined experimentally. We found that, in general, higher dimensional geometries are more stable than lower dimensions (i.e., 1-dimension or 2-dimension). Calculations for the Fe dimer yield a bond length of 1.98 angstroms, which appears to agree with experimental values (1.87 angstroms [1]). The most stable Fe trimer is an isosceles triangle. The stable geometry for n=4 is a tetrahedron. For Fe₄ and Fe₅, the stable geometries are trigonal bipyramidal and octahedral, respectively. The average magnetic moment per atom is 2.5-3.0 Bohr magnetons; this result is in agreement with previous theoretical results. Potential future work includes studies of Fe clusters with n>8, IR vibrational spectra calculations, and studies of Fe clusters encapsulated by C₆₀ fullerene.

Methods

First-principles total energy calculations were performed using density functional theory as implemented in the Vienna ab initio simulation package (VASP) [2]. The exchange–correlation energy was calculated using the generalized gradient approximation (GGA) with the parametrization of Perdew and Wang (PW91) [3]. The interaction between valence electrons and ionic cores was described by the projector augmented wave (PAW) method [4]. The Kohn–Sham equation was solved using the blocked Davidson iterative matrix diagonalization scheme, followed by the residual vector minimization method. The plane-wave cutoff energy for the electronic wavefunctions was set to a value of 500 eV.

Results and Discussion

For each cluster, we compared the total energies of the possible structures. The structure with the lowest energy is the most stable structure. The following figures illustrate the various structures and their respective total energies.

A more in-depth investigation of the stable structures reveals their magnetic moments. These findings are illustrated in the following figures.

Our calculated second energy differences deviate from the findings of Dieguez, et al. [8], who did not find any magic numbers below n=7, whereas our results indicate that the trigonal bipyramid (n=5) is a stable structure (See Fig. 5). Our calculated magnetic moments is agree with the experimental results of Billas et al. [9], which state that the average magnetic moments per atom of small Fe clusters oscillate around 3 Bohr magnetons and converge to the bulk value slowly (See Fig. 6).

Conclusions

- Average magnetic moment calculations are relatively consistent with previous findings. Further investigation is necessary, however, for larger clusters than n=8.
- The calculated bond length of the Fe dimer is 1.98 angstroms, which appears to agree with experimental values.
- Binding energies follow the same trend as previous results. Our results closely match those of Yu et al. [5].
- Energy difference between one-dimension and two-dimension seems to decrease as the number of atoms in the cluster increases.
- Energy difference between consecutive stable structures remains constant for n=8.
- Our findings for stable structures are in accord with intuition: three-dimensional structures with closer packing are stable.

Future Work

Potential future work includes studies of Fe clusters with n>8, IR vibrational spectra calculations, and studies of Fe clusters encapsulated by C₆₀ fullerene nanocontainers. Also, some of the calculated results are counter-plane-wave. For example, because Fe is very ferromagnetic, we expected all atoms to be spin-up. Some atoms in the clusters studied, however, turned out to be spin-down. Further investigation is necessary to settle this issue.

References


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