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A Molecular Dynamics Study of the Static Structure, Thermodynamic and Transport Properties of Liquid Iron Using the Modified Analytic Embedded Atom Method

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Abstract: Using the modified analytic embedded atom method (MAEAM), we have carried out molecular dynamics (MD) simulation to compute structure,thermodynamic and transport properties of liquid iron. The Foiles type effective pair potential based on the MAEAM potential functions proposed by Quyang and co-workers are shown to predict the pair distribution function well near its melting. The calculated thermodynamic properties such as, the internal energy, Helmholtz free energy and entropy are in a good agreement with experimental data. The results for the computed self-diffusion coefficients are in reasonable agreement with experiments and other works.

Key Words: liquid iron, modified analytic embedded atom method, molecular dynamics.

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