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Volume 7, No. 3, September 2007, Pages 278-303 PDF(916 KB) doi: 10.4209/aaqr.2006.09.0016 Molecular Dynamics Study of Nanoparticle Collision with a Surface

Theoretical chemistry - simple english wikipedia,

Theoretical chemistry uses The application of quantum mechanics to chemistry Computational Molecular dynamics Application of classical mechanics

Lammps - official site

LAMMPS Molecular Dynamics Simulator lamp: a device that generates light, heat, or therapeutic radiation; something that illumines the mind or soul-- www.dictionary

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