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MD Simulation for Microscale Heat Transfer

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1. Microscale Heat Transfer

1.1 Why do we deal with Molecular Dynamics?

1.2 Molecular Dynamics Method and Monte Carlo Method

1.3 Quantum Dynamics, *ab initio* Calculations

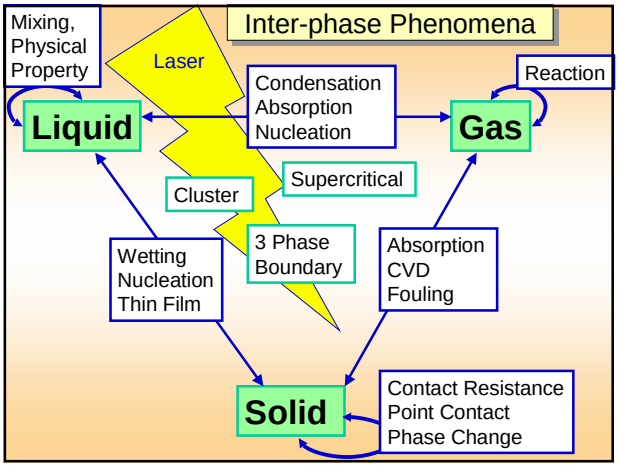
1. Microscale Heat Transfer and MD Simulation?

Fields of Applications of Molecular Heat Transfer

Heat and Mass Transfer through Interphase
(Phase Change, Ablation)
Stress at Composite Materials
Seeking for a New Materials (Especially Thermal Properties)
Manufacturing Process of Thin Film (CVD, etc)
Physical Properties of Thin Film
Fauling of Solid Materials
Numerical Prediction of Physical Properties
High Speed and High Flux Energy Transfer
Control of Cluster

Thermal Phenomena including Chemical Reactions
Manufacturing and Control with Laser,
Electron Beam and Molecular Beam

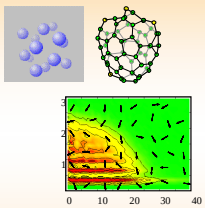
Quantum Effectn & State of Electron



Phase change phenomena

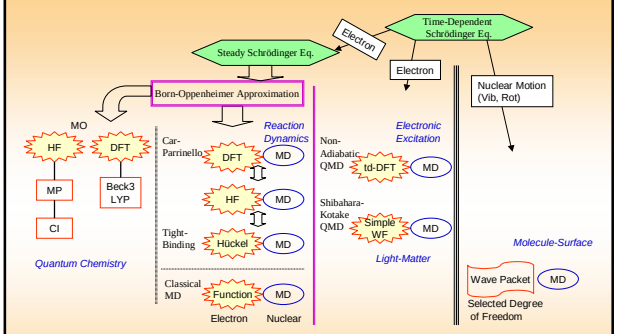
Microscopic Problems

- Clustering
- Ultra-super cooling/heating
- Uniform phase change
- Ultra-fast phase change

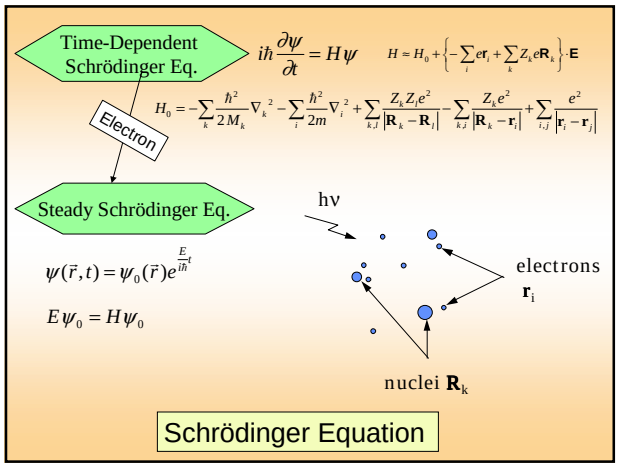


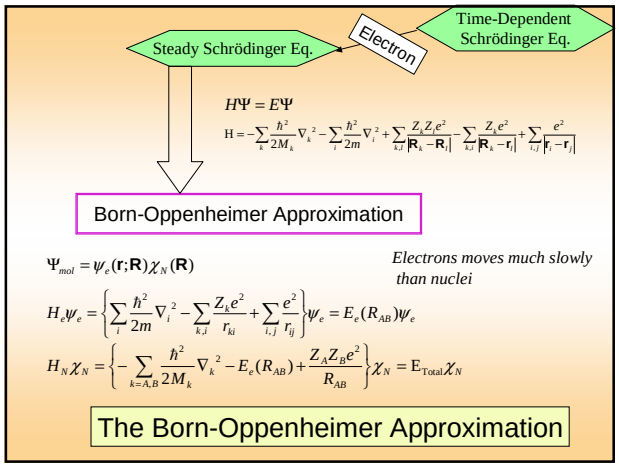
Macroscopic Problems

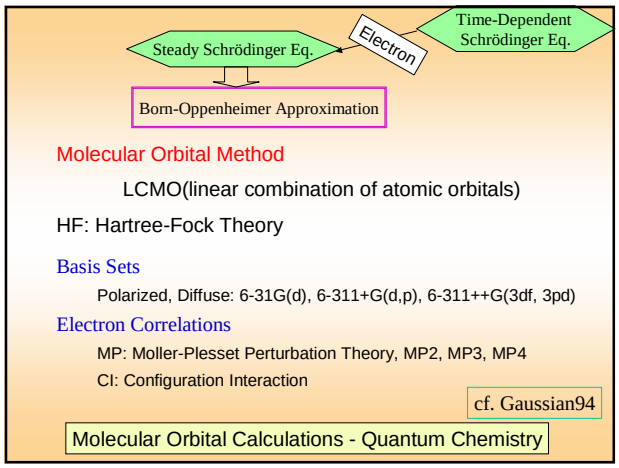
- Nucleation (homogeneous & heterogeneous)
- Maximum heat flux
- Condensation coefficient

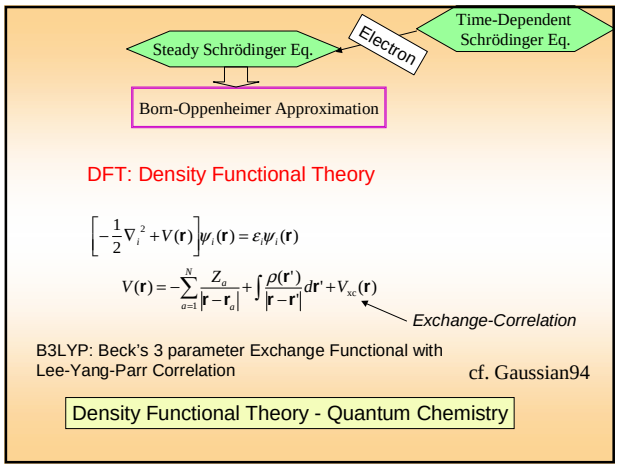


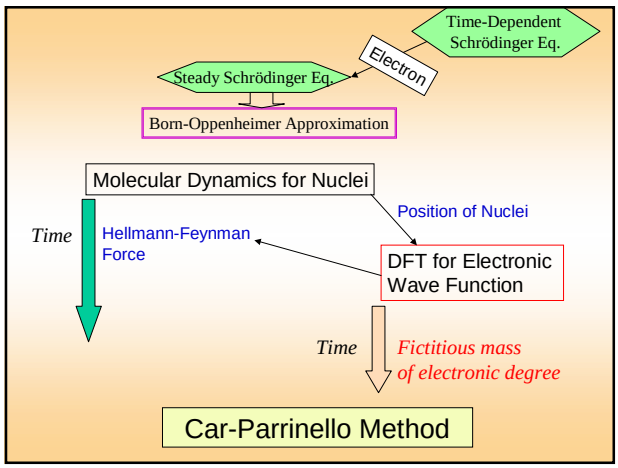
A Classification of Quantum Molecular Dynamics Methods


Time-Dependent Schrödinger Eq.
$i\hbar\frac{\partial\psi}{\partial t}=H\psi$
$H=H_0+\left\{-\sum_i e\mathbf{r}_i+\sum_k Z_k e\mathbf{R}_k\right\}\cdot\mathbf{E}$
Electron
$H_0=-\sum_k\frac{\hbar^2}{2M_k}\nabla_k^2-\sum_i\frac{\hbar^2}{2m}\nabla_i^2+\sum_{k,l}\frac{Z_k Z_l e^2}{|\mathbf{R}_k-\mathbf{R}_l|}-\sum_{k,i}\frac{Z_k e^2}{|\mathbf{R}_k-\mathbf{r}_i|}+\sum_{i,j}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}$
Steady Schrödinger Eq.
$\psi(\vec{r},t)=\psi_0(\vec{r})e^{\frac{E}{i\hbar}t}$
$E\psi_0=H\psi_0$
hν
electrons $\mathbf{r}_i$
nuclei $\mathbf{R}_k$
Schrödinger Equation


Steady Schrödinger Eq.
Electron
Time-Dependent Schrödinger Eq.
$H\Psi=E\Psi$
$H=-\sum_k\frac{\hbar^2}{2M_k}\nabla_k^2-\sum_i\frac{\hbar^2}{2m}\nabla_i^2+\sum_{k,l}\frac{Z_k Z_l e^2}{|\mathbf{R}_k-\mathbf{R}_l|}-\sum_{k,i}\frac{Z_k e^2}{|\mathbf{R}_k-\mathbf{r}_i|}+\sum_{i,j}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}$
Born-Oppenheimer Approximation
$\Psi_{mol}=\psi_e(\mathbf{r};\mathbf{R})\chi_N(\mathbf{R})$
Electrons moves much slowly than nuclei
$H_e\psi_e=\left\{\sum_i\frac{\hbar^2}{2m}\nabla_i^2-\sum_{k,i}\frac{Z_k e^2}{r_{ki}}+\sum_{i,j}\frac{e^2}{r_{ij}}\right\}\psi_e=E_e(R_{AB})\psi_e$
$H_N\chi_N=\left\{-\sum_{k=A,B}\frac{\hbar^2}{2M_k}\nabla_k^2-E_e(R_{AB})+\frac{Z_A Z_B e^2}{R_{AB}}\right\}\chi_N=\mathrm{E}_{\mathrm{Total}}\chi_N$
The Born-Oppenheimer Approximation


Steady Schrödinger Eq.
Electron
Time-Dependent Schrödinger Eq.
Born-Oppenheimer Approximation
Molecular Orbital Method
LCMO(linear combination of atomic orbitals)
HF: Hartree-Fock Theory
Basis Sets
Polarized, Diffuse: 6-31G(d), 6-311+G(d,p), 6-311++G(3df, 3pd)
Electron Correlations
MP: Moller-Plesset Perturbation Theory, MP2, MP3, MP4
CI: Configuration Interaction
cf. Gaussian94
Molecular Orbital Calculations - Quantum Chemistry


Steady Schrödinger Eq.
Electron
Time-Dependent Schrödinger Eq.
Born-Oppenheimer Approximation
DFT: Density Functional Theory
$\left[-\frac{1}{2}\nabla_i^2+V(\mathbf{r})\right]\psi_i(\mathbf{r})=\varepsilon_i\psi_i(\mathbf{r})$
$V(\mathbf{r})=-\sum_{a=1}^{N}\frac{Z_a}{|\mathbf{r}-\mathbf{r}_a|}+\int\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'+V_{xc}(\mathbf{r})$
Exchange-Correlation
B3LYP: Beck's 3 parameter Exchange Functional with Lee-Yang-Parr Correlation
cf. Gaussian94
Density Functional Theory - Quantum Chemistry


Steady Schrödinger Eq.
Electron
Time-Dependent Schrödinger Eq.
Born-Oppenheimer Approximation
Molecular Dynamics for Nuclei
Position of Nuclei
Time
Hellmann-Feynman Force
DFT for Electronic Wave Function
Time
Fictitious mass of electronic degree
Car-Parrinello Method