First Principles Molecular Dynamics Analysis on the Molten Electrolytes of Thermal Batteries

熱電池電解質-熔融鹽混合物之第一原理分子動力學模擬分析

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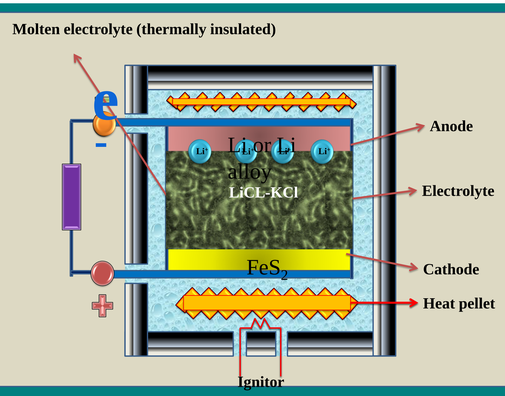
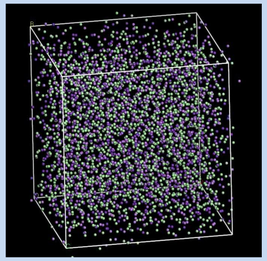
Objective

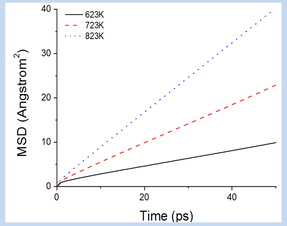
(1) Thermal Batteries Molten Electrolytes
(2) Classical Molecular Dynamics
(3) First Principles Molecular Dynamics
(4) Ionic Conductivity, Thermal Conductivities,
(5) Melting Points

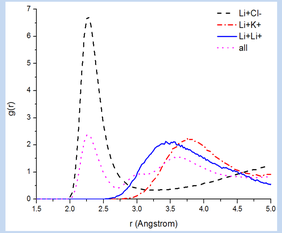


Result and discussion

MD

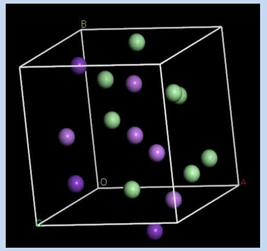


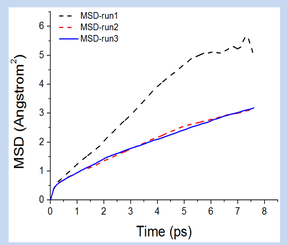


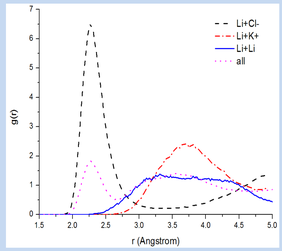


Mean square displacement Radial distribution function

FPMD

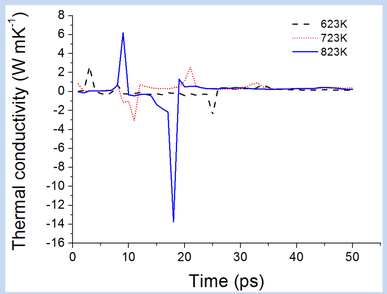




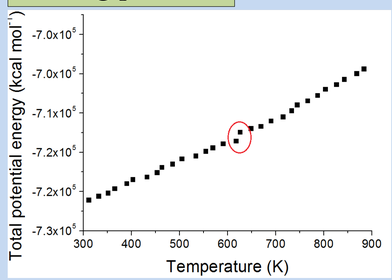


Mean square displacement Radial distribution function

RNEMD



Melting point



Theory

Molecular Dynamics, MD

$$\vec{F} = -\nabla U$$

$$U_{intra} = U_{bond} + U_{angle} + U_{dihedra} + U_{inversion}$$

$$\vec{F} = m\vec{a} = m\frac{d^2x}{dt^2}$$

$$\vec{v} = \int \vec{a}dt \qquad \vec{x} = \int \vec{v}dt$$

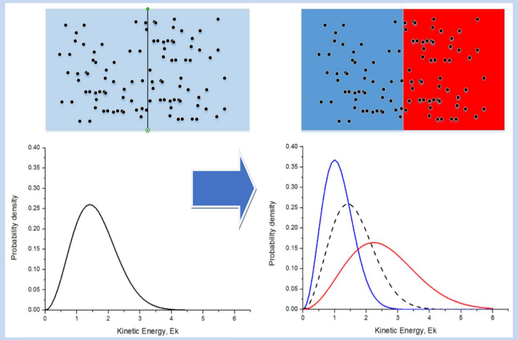
DFT and First Principles Molecular Dynamics (FPMD)

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V_n(r) + V_H(r) + V_{xc}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r)$$

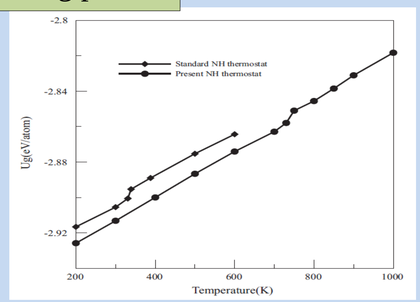
$$\frac{dE}{d\lambda} = \left\langle \psi(\lambda)\left|\frac{dH(\lambda)}{d\lambda}\right|\psi(\lambda)\right\rangle = \nabla\left\langle \psi(\lambda)|H|\psi(\lambda)\right\rangle = -\vec{p}_i$$

$$M_I\ddot{R}_I(t) = -\nabla_I\left\{\min_{\psi}\left\langle \Psi_0|H_e|\Psi_0\right\rangle\right\}$$

Revered non-equilibrium molecular dynamics, RNEMD



Melting point



Simulation steps