Multiscale Multiphysics Simulation Model of Laser-Induced Ultrasonic Energy Conversion

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Introduction

Laser-induced ultrasound showcases its peculiarities on **wide-bandwidth high-central frequency** ultrasound generation to realize rapid detection and high resolution of all-optical intravascular ultrasound imaging and diagnosis. The exceptional performance comes form its complicated interaction of **energy conversion**.

A **multiscale multiphysics simulation** model describing **laser-induced ultrasonic energy conversion** is needed to properly control the laser dose and design structured absorbers.

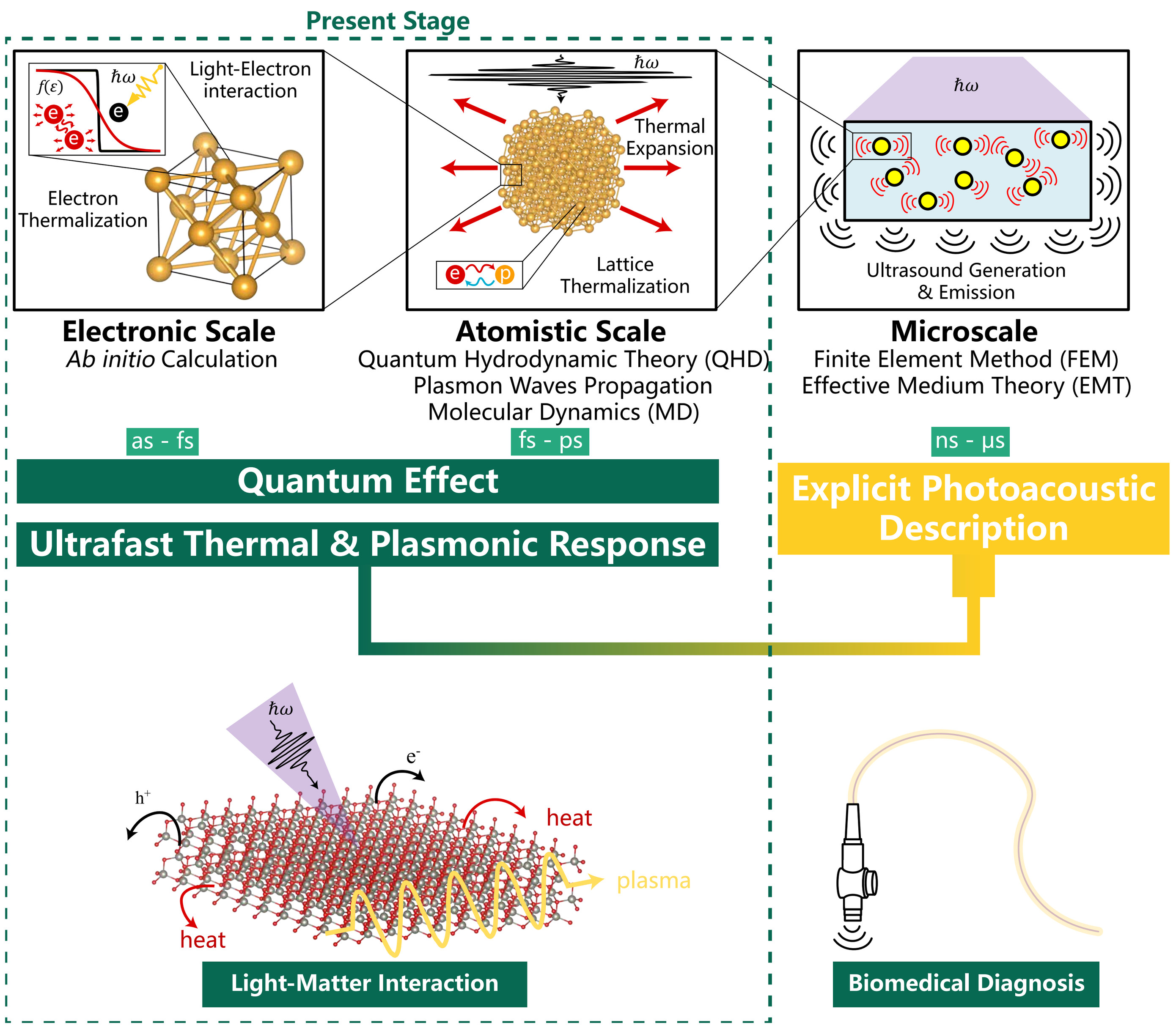

Figure 1. Schema of Multiscale Multiphysics Simulation Model of Laser-Induced Ultrasonic Energy Conversion

Numerical prediction model for femtosecond laser excitation response of gold nanoparticles.

Bridging Electronic and Atomistic

- **Ultrafast Thermal Response** is captured in Electronic Scale model, as **thermal properties at electronic excited states**, as well as **lattice thermalization by electron-phonon coupling** in Atomistic Scale model
- **Plasmonic Response** is captured in Atomistic Scale model, coupled with **Maxwell's Equations** as electromagnetic wave propagation

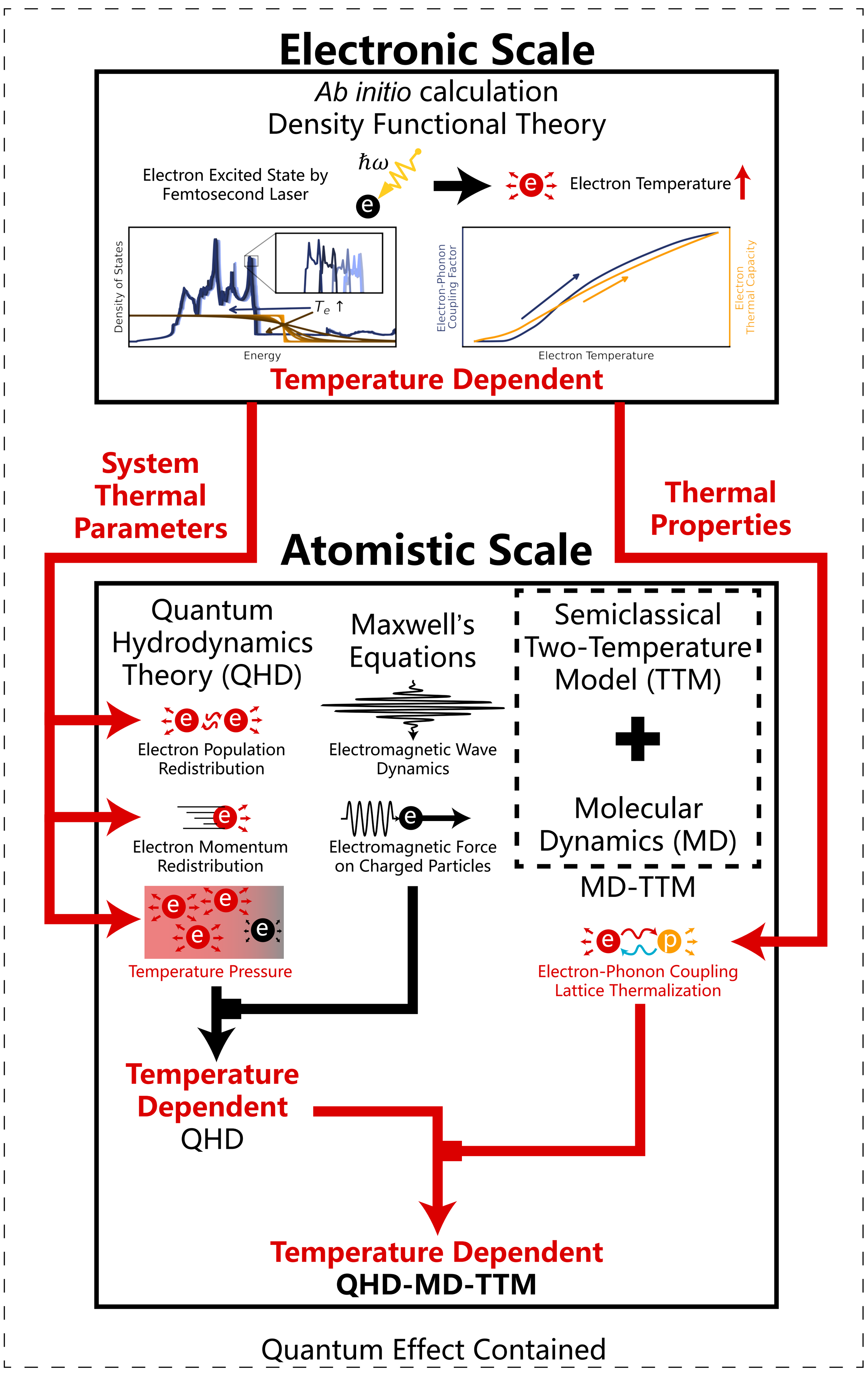

Figure 2. Workflow of Simulation Model Bridging Electronic Scale and Atomistic Scale

Electron excited states by femtosecond laser are imitated to predict electron temperature dependent system thermal parameters and thermal properties, as Electron Scale model [1]. By using them, Quantum Hydrodynamics Theory with Maxwell's Equations [2] and Semiclassical Two-Temperature Model with Molecular Dynamics [3,4] are united as Atomistic Scale model.

Performing Atomistic Scale Model

- **First-order perturbation and relaxation time approximation**
- **1-D model** for simplification

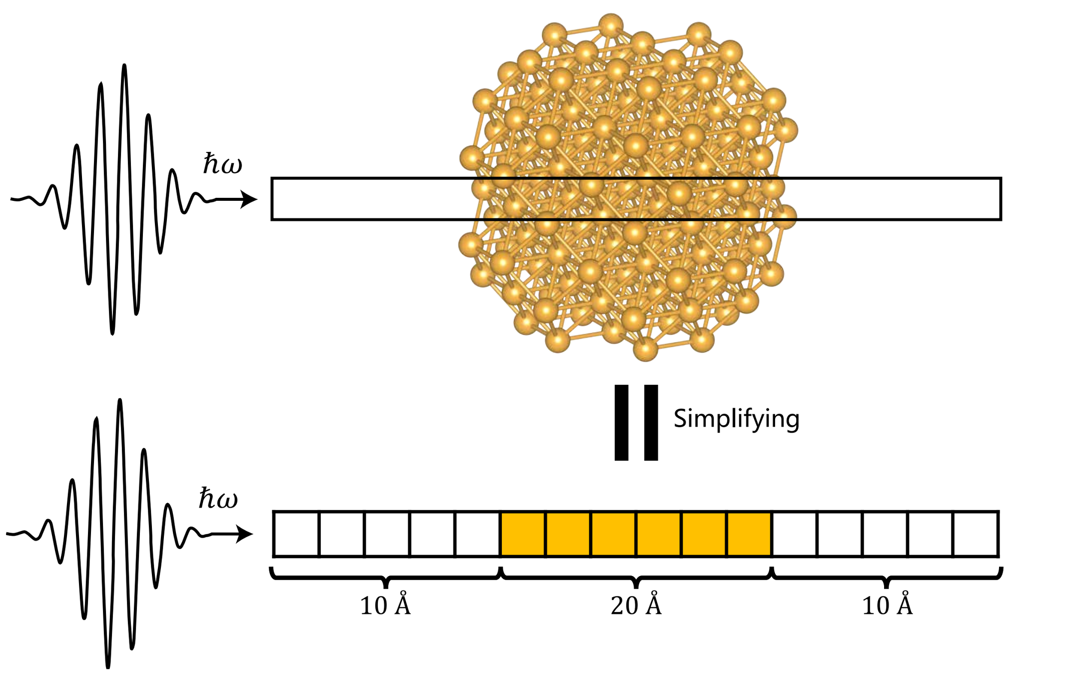

Figure 3. 1-D Model Simplification and Discretization

1-D model was used as preliminary research and modeling

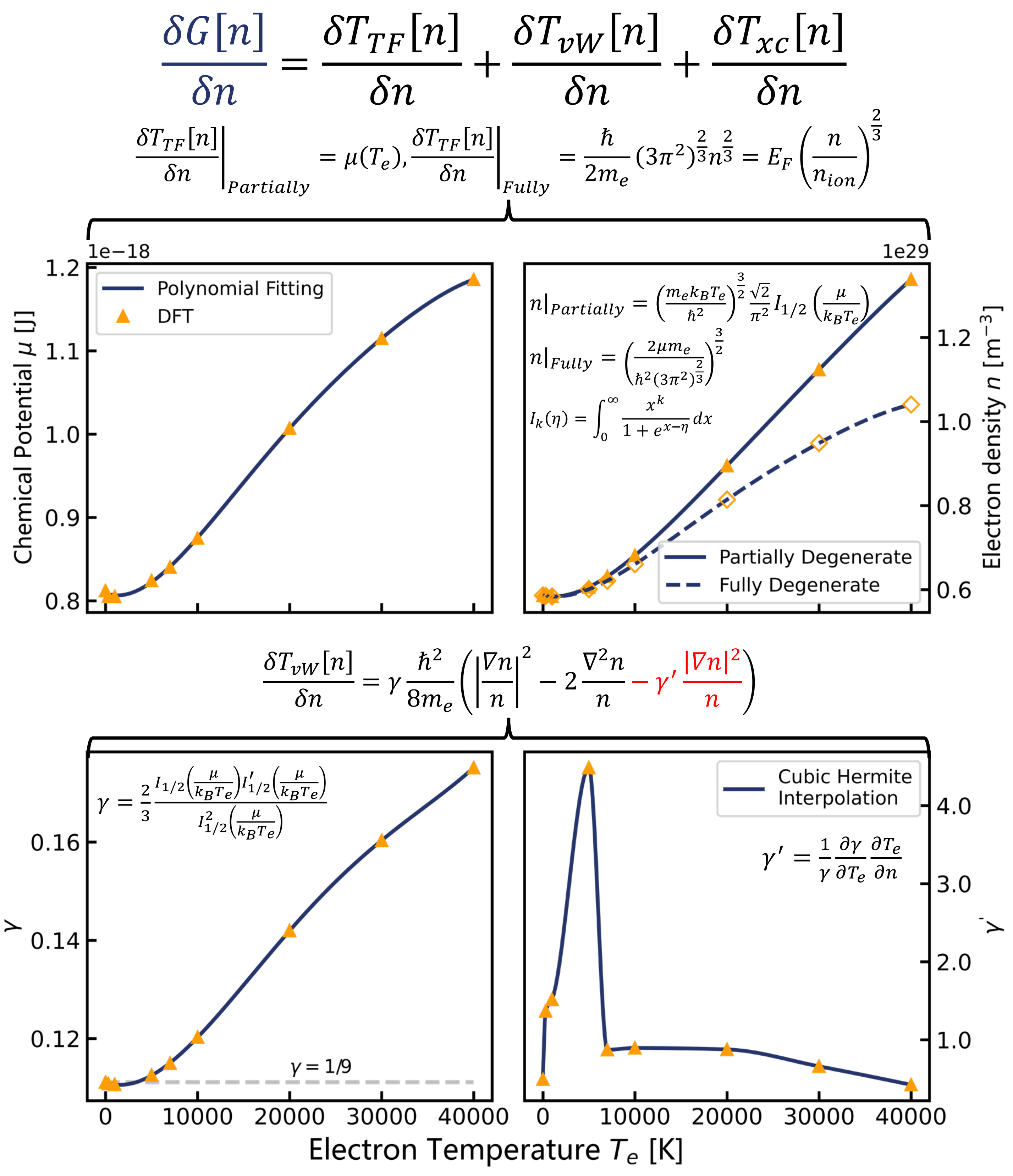

Figure 4. Coefficients Evolution in Quantum Energy Term

Quantum energy term in Quantum Hydrodynamics Theory is given at the top.
(up) Thomas-Fermi kinetic energy based on Local Density Approximation and Fermi statistic, considering chemical potential and free energy density at fully degenerate and partially degenerate description.
(down) von Weizsäcker gradient correction of kinetic energy, with two electron temperature dependent coefficients γ and γ', the latter often be ignored.

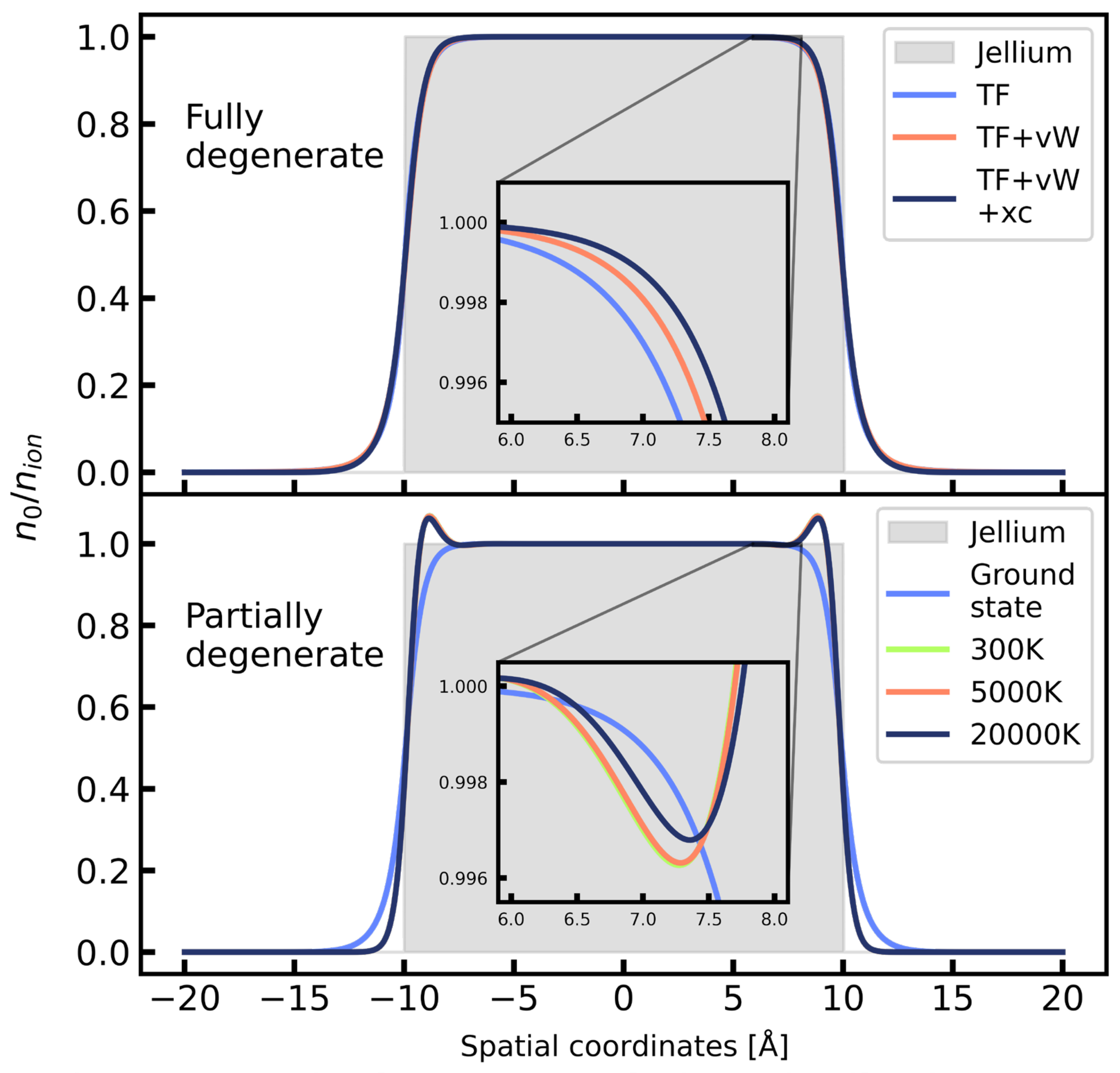

Figure 5. Static Electron Population Distribution

(up) Fully degenerate quantum energy term with functionals, indicating ground state.
(down) Partially degenerate quantum energy term at varying electron temperature. Both showed apparent electron spill-out effect and its dependence on electron temperature.

Future Plan

- **Time dependent** electron distribution with Atomistic Scale model, to obtain **plasmonic response and thermal effect**
- **Time dependent** electron-lattice and dopant-environment **energy transfer**
- Extending to 2-D and 3-D model

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Reference

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