Abstract Submitted
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***Ab initio* molecular dynamics study of liquid Li and interactions with deuterium and tritium** MOHAN CHEN, Princeton University, EMILY CARTER, Princeton Universtiy — We investigate the structure of liquid Li and its interaction with deuteriumand tritium atoms using PROFESS (PRinceton Orbital-Free Electronic Structure Software) [1]. This linear-scaling orbital-free density functional theory method is a very fast quantum mechanics technique that allows one to perform ab initio molecular dynamics of metals for a large number of atoms and fairly long time. We predict 434 K as the melting temperature of Li [2], which compares well with an experimental melting point of 453 K [3]. Key properties of liquid Li will be presented and discussed, such as its diffusion coefficients and static structure factors, etc. We will also present some preliminary results of simulations of deuterium and tritium atom adsorption on liquid L. This work provides new insights into understanding the bulk and surface structure and reactivity of liquid Li using large-scale ab initio molecular dynamics methods.

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