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Abstract for an Invited Paper
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Ab initio modelling of the transport and solvation of positrons in dense gases and liquids[1]

DANIEL COCKS, Australian National University

I will contrast the modelling of the transport of electrons and positrons through dilute gases with the formalism required for modelling the same transport through dense fluids. In dilute gases, this is well described by the Boltzmann equation and easily accessible to particle-track Monte Carlo simulations. The major impediment to accurate simulation predictions lies in the determination of accurate cross section sets. In contrast, the accurate simulation of dense fluids, including liquids and dense gases, provide challenges for ab initio calculations in the form of screening effects, interference, self-trapping and collective excitations. This talk will overview our progress towards a complete ab initio model for transport in dense fluids, and describe the requirements to include solvation as a Monte Carlo process. A key parameter, V_0, the minimum of the conduction band, lies at the heart of understanding transport in liquids. While experiments to determine V_0 for electrons in dense fluids can be implemented through photo- or field-ionization, these processes are unavailable to positrons and so direct measurement V_0 is unlikely to be performed. Hence, theoretical models are crucial and I present an ab-initio prediction of $V_0(n_0)$, where n_0 is the fluid density, for positrons in noble-gas gases and liquids. I will show how this result can be applied in transport calculations to determine lifetimes. Finally, I will show how the extension to address dense fluids of polar molecules can easily be described, by formally including molecule orientation. However, the implementation of this extension causes considerable difficulty in both the identification of natural fluctuations in the bulk and the use of appropriate structure information of the fluid. I will discuss different techniques for addressing these issues.

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