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Excited-state PAW Potentials: Modelling Hot-Dense Plasmas From First Principles PATRICK HOLLEBON, SAM VINKO, ORLANDO CIRICOSTA, JUSTIN WARK, University of Oxford — Finite temperature density functional theory has proven to be a successful means of modelling warm and hot dense plasma systems, including the calculation of transport properties [1], equation of state [2] and ionization potential depression [3]. Such methods take into account the non-negligible influence of quantum mechanics on the electronic structure of these strongly coupled systems. We apply excited state frozen core potentials to model general core-hole states in high density plasma, allowing for the calculation of the electronic structure of a range of ionic configurations. The advantages of using excited-state potentials are explored and we investigate their application towards various response function calculations, with the results shown to be in good agreement with all-electron calculations at finite-temperatures.

[1] F. Lambert *et al.*, Physics of Plasmas, **18**, 056306 (2011).
[2] Jean Clérouin *et al.*, Phys. Rev. B **71**, 064203 (2005).
[3] S.M. Vinko *et al.*, Nat. Commun, 5:3533 (2014).

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