Excited-state PAW Potentials: Modelling Hot-Dense Plasmas
From First Principles

PATRICK HOLLEBON, SAM VINKO, ORLANDO CIRI-COSTA, 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.