

# Pseudoatom Molecular Dynamics Plasma Microfields

J. R. White<sup>\*1,2</sup>, C. J. Fontes<sup>2</sup>, M. C. Zammit<sup>2</sup>, T. A. Gomez<sup>1,3,4</sup>, C. E. Starrett<sup>2</sup>

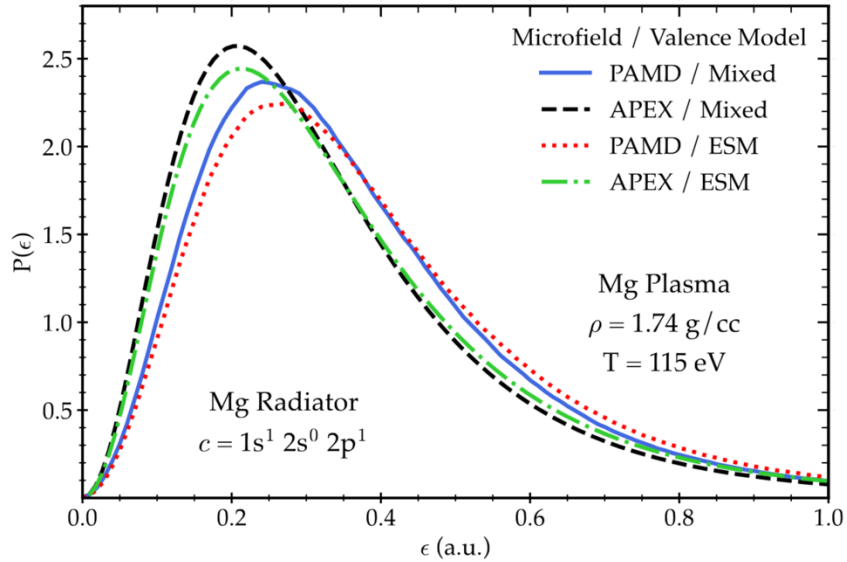
<sup>1</sup>Department of Astronomy, University of Texas at Austin, Austin TX, USA

<sup>2</sup>Los Alamos National Laboratory, Los Alamos NM, USA

<sup>3</sup>Astrophysical and Planetary Sciences, University of Colorado Boulder, Boulder CO, USA

<sup>4</sup>National Solar Observatory, University of Colorado Boulder, Boulder CO, USA

Spectral line profiles are powerful diagnostic tools for both laboratory and astrophysical plasmas, as their shape is sensitive to the plasma environment. The low-frequency component of the electric microfield is an important input for analytic line broadening codes. In this poster we present a new method of calculating plasma microfields using configuration-resolved pseudoatom molecular dynamics. This approach accounts for both quantum atomic structure and N-body effects, similar to density functional theory molecular dynamics, but with less computational cost. We present pseudoatom microfields at conditions relevant for recent laboratory experiments. Compared to established microfield codes we find moderate deviations at solid density conditions and strong agreement at lower plasma densities.



**Figure 1.** Microfields in a solid-density Mg plasma for an excited He-like Mg atom [1]. The PAMD results (this work) are compared to the APEX code [2]. Different treatments of the valence shell, one following the Excited State Model [3] (ESM) and one following a mixing procedure are compared.

## References

- [1] J. R. White, C. J. Fontes, M. C. Zammit et al., <https://arxiv.org/abs/2407.14455>
- [2] C. A. Iglesias, F. J. Rogers, R. Shepherd et al., *JQSRT* **65**, 303–315 (2000)
- [3] C. E. Starrett, T. Q. Thelen, C. J. Fontes et al., *PRE* **109**, 035201 (2024)

\* E-mail: jacksonw@lanl.gov