Focus Session

New Theoretical Approaches to Collisions and Specroscopy

2:00 pm – 4:00 pm, Tuesday June 17 // Session C07 //

Oregon Convention Center, E141-142

Chair: Jesús Pérez-Ríos, Stony Brook University (SUNY)

Topics: Atoms; Charged Particles; Interactions; Ions; Molecules ... Show all topics

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The Opacity Project: R-matrix calculations, plasma broadening effects and equation-of-State for High-Energy-Density sources

3:12 pm – 3:24 pm

Presenter: Divya Chari (The Ohio State University)

Authors: Anil Pradhan (Ohio State University), Sultana Nahar (Ohio State Univ - Columbus)

Accurate opacity calculations are critical for understanding radiation transport in both astrophysical and laboratory plasmas. We employ atomic data from R-Matrix calculations to investigate radiative properties in high-energy-density (HED) sources, focusing on opacity variations under extreme plasma conditions. Specifically, we analyze environments such as the base of the convective zone (BCZ) of the Sun (2×10^6 K, 10^{23} cm^{-3}), and radiative opacity experiments conducted at inertial confinement fusion (ICF) devices at the Sandia Z

facility (2.11×10^6 K, 3.16×10^{22} cm^{-3}), and the Lawrence Livermore National Laboratory National Ignition Facility. We calculate Rosseland Mean Opacities (RMO) within a range of temperatures and densities and analyze how they vary under different plasma conditions. A significant factor influencing opacity in these environments is line and resonance broadening due to plasma effects. Both radiative and collisional broadening modify line shapes, impacting the absorption and emission profiles that determine the RMO. We specifically utilize a new methodology for plasma effects on autoionizing resonances due to electron collisional, Stark ion microfield, and other broadening effects in HED plasmas. We assume a Lorentzian profile factor to model combined broadening and investigate its impact on spectral line shapes, resonance behavior, and overall opacity values. Our results are relevant to astrophysical models, particularly in the context of the solar opacity problem, and provide insights into discrepancies between theoretical calculations and experimental measurements. In addition, we investigate the equation-of-state (EOS) and its impact on opacities. In particular, we examine the "chemical picture" Mihalas-Hummer-Dappen EOS with respect to level populations of excited levels included in the extensive R-matrix calculations. This study contributes to improving opacity models used in stellar structure calculations and laboratory plasma experiments.

PRESENTATIONS (7)

Filter presentations

2:00 pm – 2:30 pm
Machine learning approaches to extend and improve state-resolved molecular collision data
Robert C Forrey (presenter), Darin Mihalik, Ruihan Wang, Benhui Yang, Phillip Stancil, T. J. Price, N. Balakrishnan, Roman V Krems

2:30 pm – 3:00 pm
Data-Driven Machine Learning Models for Atomic and Molecular Collisions
Allison L. Harris (presenter)

3:00 pm – 3:12 pm
Accelerating Monte Carlo Simulation of Rare Events by Importance Sampling using Neural Network
Myung Chul Kim (presenter), Wei Cai

3:12 pm – 3:24 pm
The Opacity Project: R-matrix calculations, plasma broadening effects and equation-of-State for High-Energy-Density sources
Divya Chari (presenter), Anil Kumar Pradhan, Sultana Nurun Nahar

3:24 pm – 3:36 pm

The Los Alamos National Laboratory MOLecular OPacity (MOLOP) Suite of Codes – Application to Air Plasma

Amanda Joy Neukirch (presenter), Mark C Zammit, Isuru Ariyarathna, James P Colgan, Christopher J Fontes, Aaron Forde, Jeffery A Leiding, Eddy M Timmermans

3:36 pm – 3:48 pm

Comparing theoretical methods of electron molecular-ion scattering with a hydrogen-like toy model

David Hvizdos (presenter), Chris H Greene, Roman Curik, Ioan F Schneider, Zsolt Z Mezei

3:48 pm – 4:00 pm

The global potential energy surface and sticking time of the AlF dimer

Mahmoud A Ibrahim (presenter), Xiangyue Liu, Weiqi Wang, Jesús Pérez-Ríos

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