SALSAA: Statistically Averaged Line Shapes from Average Atom

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We report on an approach to computing ion-Stark contributions to line shapes based on self-consistent data from an average-atom model. The average-atom model uses density functional theory (DFT) to generate Kohn-Sham orbitals for electrons in a self-consistent electron-ion potential within a neutral ion sphere. The free-electron part of the electron distribution is used along with a response function to produce an ion-ion potential that defines a self-consistent radial distribution function and nearest-neighbor distribution for the ions. In traditional approaches to line-broadening, the ion distribution would be used to generate an electric field distribution which, coupled with perturbation theory for the response of bound states to electric microfields, provides the ion-Stark contribution to emission and absorption line broadening. In SALSAA, perturbations in electron binding energies are computed due to changes in the nearest-neighber location and convolved with the self-consistent nearest-neighbor distribution function to generate the ion-Stark contribution to line broadening. This presentation will compare each part of the new method to traditional calculations, showing that the statistical approach can reproduce many of the features of traditional methods with high computational efficiency, enabling self-consistent estimates of ion-Stark line broadening in multi-electron ions.

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