Molecular Dynamics Investigation of the Ion Migration of Inorganic Metal Halide Perovskites

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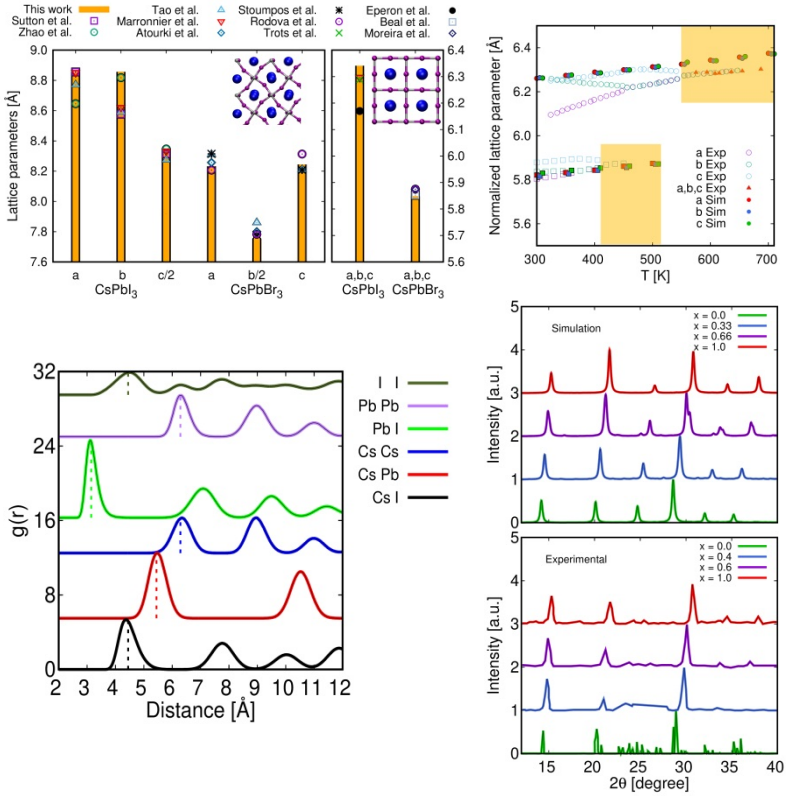
The comprehensive description of the ion migration in metal halide perovskites (MHPs) is important to understand the performance of perovskites solar cells. We use classical molecular dynamics (CMD) simulations to obtain structural properties of MHPs and the dynamics of halide vacancies.

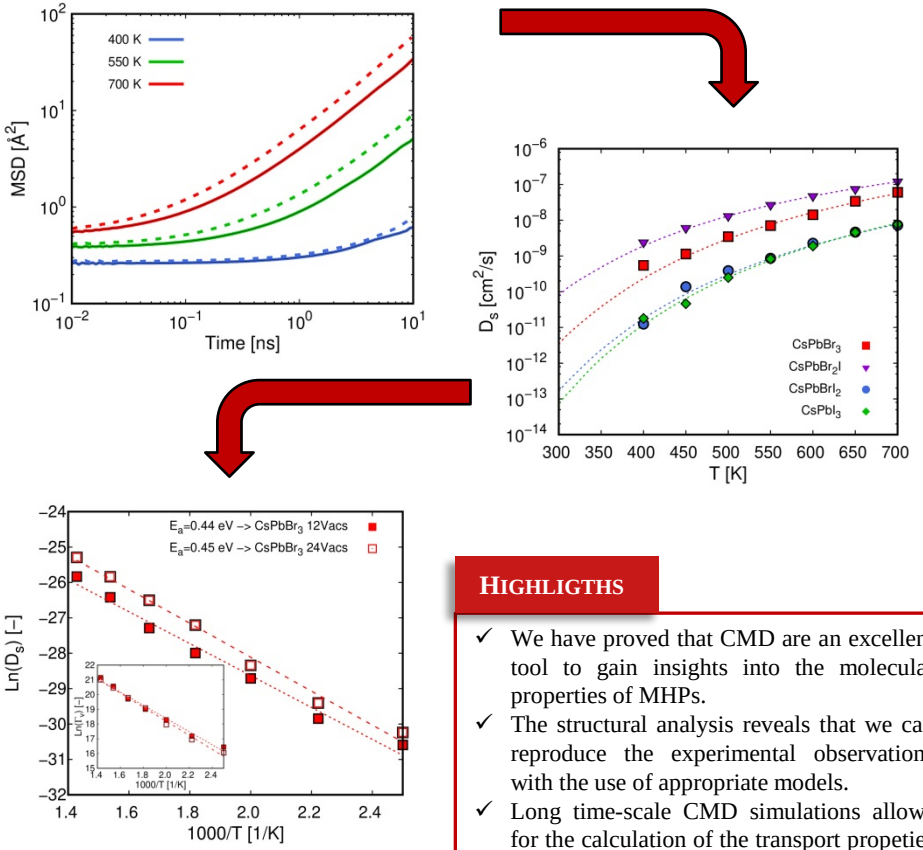
Structural properties

Comparison between experimental and computed lattice parameters, interatomic distances, and XRD spectra of $CsPbX_3$ (X = I, Br) MHPs.



Dynamical properties

Mean squared displacement, self diffusion coefficients, activation energies, and jump rates of halide vacancies in mixed $CsPb(Br_xI_{1-x})_3$ perovskites



Highligths

- ✓ We have proved that CMD are an excellent tool to gain insights into the molecular properties of MHPs.
- ✓ The structural analysis reveals that we can reproduce the experimental observations with the use of appropriate models.
- ✓ Long time-scale CMD simulations allows for the calculation of the transport propeties of halide vacancies in pure and mixed MHPs.