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**Understanding thermally activated phenomena in hybrid organic-inorganic halide perovskites by molecular dynamics simulations.**

# Alessandro Mattoni

**Development of classical force fields for thermal transport in methylammonium lead halide.**

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# Understanding thermally activated phenomena in hybrid organic-inorganic halide perovskites by molecular dynamics simulations

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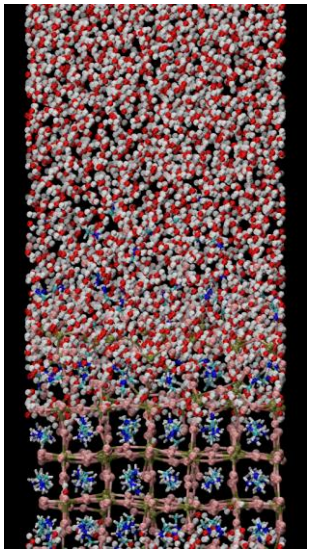

The success of hybrid lead halide perovskites in the field of photovoltaics has given rise to an intense research effort to study its fundamental properties. These hybrid materials with general formula $ABX_3$ are formed by organic cations occupying the A sites within an inorganic lead halide $PbI_3$ sublattice. From a fundamental perspective, they are hybrid crystals representing an ideal paradigm to understand hybrid interactions in ionic materials.

The electronic levels of the molecules are not directly involved in the optoelectronic processes of the material and the intrinsic recombination and photovoltaic activity of the crystal can be almost correspond to an inorganic semiconductor with a hybrid body [1,2]. However, the actual molecular orientations have an impact on the distortions of the inorganic lattice and, in turn, on the electronic and transport properties [2]. At finite temperature, the interplay between the rotational dynamics of the molecules and the inorganic lattice is important to understand the relaxation processes and the molecular order within the material.

Here, we discuss the development of an ionic interatomic model [3] with reduced computational cost and to its application to study dynamical properties of the hybrid perovskites [4]. The model makes possible to study the molecular reorientational times, calculated under controlled thermodynamic conditions, spanning from the orthorhombic to the cubic phase. Furthermore, it opens the way to the large-scale atomistic simulations of dynamical processes in hybrid perovskites and its nanostructures. We discuss applications including infrared absorption[4], point-defects mobility, thermal transport, and degradation of hybrid perovskites in water.

**References**

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Short bio

Alessandro Mattoni is staff researcher at the Cagliari Unit of Istituto Officina dei Materiali (CNR-IOM) where he coordinates the theoretical research on nanomaterials for energy. A.M. graduated in Physics at the University of Perugia in 1998, earned his PhD in Physics at the University of Padova and moved to Department of Physics of the University of Cagliari in 2003 working at the Sardinian Laboratory for Computational Materials Science and, since 2010, as a researcher of Consiglio Nazionale delle Ricerche. A.M. has a long-term expertise in atomistic simulations based on molecular dynamics and multiscale modeling of materials with applications in nanomechanics, opto- and micro-electronics, photovoltaics and photocatalysis. A.M. is author of about 80 publications in international peered-reviewed journals and reviewer for journals of ACS, APS, Wiley, and Elsevier. A.M. has been unit- coordinator of several national and international projects related to nanomaterials for energy RAS-2009, RAS-2011, MIUR-PRIN, EU-FP6, PON-Netergit. During 2010-2013 he has been the national coordinator of the IIT-SEED national project POLYPHEMO on hybrid polymer based materials for photovoltaics funded by the Istituto Italiano di Tecnologia.

# Development of classical force fields for thermal transport in methylammonium lead halide

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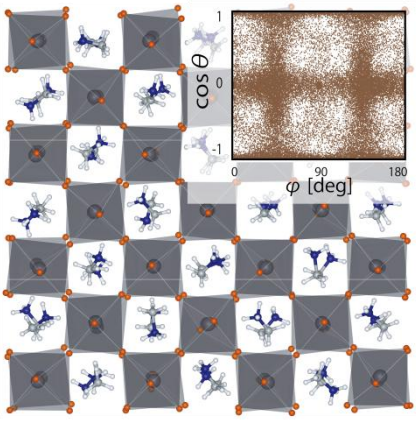
Organic-inorganic hybrid perovskites (OIHPs) have recently attracted attention for possible thermoelectric materials. In such structures, embedded molecules are expected to provide selective and tunable degrees of freedom for thermal properties. However such applications require a further understanding of the thermodynamic properties of hybrid perovskites, for which the molecular dynamics approach is very promising. A few empirical potentials have been already reported for the most typical OIHP, methylammonium lead iodide (MAPI) [1,2], but no potentials have been developed for other hybrid perovskites. Here we discuss the strategy to develop model potentials for the OIHP-family with different halides, focusing on the case of methylammonium lead bromide (MAPBr). This scheme starts from the functional form and the parameters of MAPI obtained in the previous work [2], which is detuned by fitting to the experimental/DFT data of the target material. We found that static energy properties of MAPBr can be reproduced by introducing only three scaling parameters: one for inorganic-inorganic interactions, another for organic-inorganic interactions, and the other for atomic point charges. Further refinements are required to reproduce the thermodynamic properties, such as the orthorhombic-to-tetragonal phase transition. We show that this is possible by a suitable calibration of the inorganic-organic interactions while refining the scaling parameters. The present strategy is independent on the specific halide investigated and it can be extended directly to other OIHP materials.

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Short bio

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