Società Chimica Italiana
Divisione di Chimica Inorganica

XLIX CONGRESSO NAZIONALE
DI CHIMICA INORGANICA
PERUGIA 12-15 SETTEMBRE

INORG2023

BOOK of ABSTRACTS

http://inorg2023.chm.unipg.it

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STRUCTURAL PROPERTIES DETERMINING THE NEAR-EDGE X-RAY ABSORPTION SPECTRA OF LEAD HALIDE PEROVSKITES

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X-ray absorption spectroscopy (XAS) is an excellent complement to diffraction techniques for studying the structure of materials. Despite the extensive research on lead halide perovskites for optoelectronic applications, the application of XAS to these materials has been relatively limited and yielded varying degrees of success. In order to develop generalizable approaches for analyzing XAS spectra of halide perovskites with different compositions, we conducted an experimental and computational study on a hybrid Pb/Bi iodide solid solution, serving as a model system. The monodimensional lead halide "perovskite" $(TMSO)_3Pb_{3x}Bi_{2(1-x)}I_9$[1] exhibits correlated disorder at the metal cation site, resulting in various possible arrangements of Pb, Bi, and metal vacancies (Figure 1). Through simulations, we observed that the X-ray absorption near-edge structure spectra (at the Pb, Bi, and I X-ray absorption edges) show some sensitive to these alternations. Surprisingly, we discovered that the cation spectra can be explained by simple distortions of independent PbI_6/BiI_6 octahedral units, without considering long-range multiple scattering contributions that typically dominate the near-edge region.[2] This finding enables the prediction and modeling of X-ray absorption near-edge spectra using simple structural units, suggesting that similar approaches can be successfully extended to other halide perovskites in the future.

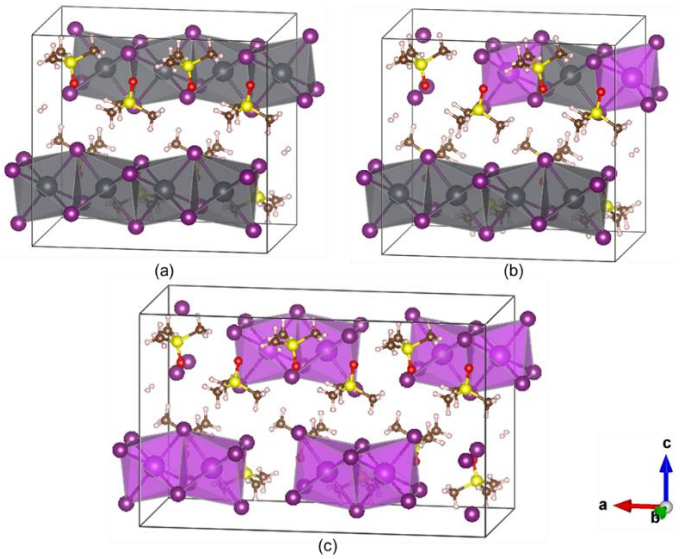

Figure 6: *(a) Undoped $TMSO_8Pb_8I_{24}$ 2 x 1 x 1 supercell. (b) Pb/Bi iodide solid solution. (c) $(TMSO)_3Bi_2I_9$supercell.*

[1] C. Pipitone, F. Giannici, A. Martorana, C. García-Espejo, S. Carlotto, M. Casarin, A. Guagliardi, N. Masciocchi, *J. Phys. Chem. C***2021**, *125*, 11728–11742.
[2] S. Virga, A. Longo, C. Pipitone, F. Giannici, submitted to *J. Phys. Chem. C* **2023**.