

MS13 Structural Characterization of Functional Materials

MS13.1-01

Crystal structure, characterization and physical properties of lead-free organic-inorganic hybrid perovskites
S. Abdel-Aal¹, A. Abdel-Rahman¹, N. Claiser², M. Souhassou², J. Martorell³, C. Lecomte²

¹Cairo university (*Egypt*), ²Lorraine university (*France*), ³ICFO (*Spain*)

Abstract

Organic- inorganic hybrid perovskites gain considerable attention recently and more studies have been done as changing the halide, metal ion or /and the ligand enables to tune the optical, electric, magnetic, ferroelectric and multiferroic properties. Halide perovskites in particular lead halides are interesting semiconductors with a direct band gap (1.5 eV) which enables collecting visible photons. These luminescent crystals have no future for safety and ecological reasons. Diammonium halide perovskite hybrids $[NH_3(CH_2)_nNH_3]MCl_xBr_{4-x}$; $x = 0, 2, 4$; $M = Co, Mn$; $n = 4-9$ allow mixing of organic and inorganic components in one molecule which possesses a property that may not exist in either of the parent components. The complete structure information as well as lattice parameters for Co series $n = 4-9$ are provided, and for $n = 3-6$ for Mn hybrid. Differential thermal analysis DSC shows reversible order - disorder transition for both the Co and Mn hybrids. Permittivity studies confirm the phase transition. The optical properties of Co series show strong absorption in the visible range, the band gap (1.73 eV) which is promising for photovoltaic applications.

References

- 1-Seham K. Abdel-Aal, A. Ouasri, "Crystal structure, Hirshfeld surfaces and vibrational studies of tetrachlorocobaltate hybrid perovskite salts $NH_3(CH_2)_nNH_3CoCl_4$ ($n = 4, 9$)" Journal of Molecular Structure , 2022, 1251, 131997
- 2-Seham. K. Abdel-Aal, A. S. Abdel-Rahman, G. Bortel, Á. Pekker, K. Kamarás, G. Faigel, "Structure investigation and vibrational spectroscopy of two prospective hybrid perovskites based on Mn and Co" Journal of Physics and Chemistry of Solids, 2022, 161, 110400
- 3-Seham K. Abdel-Aal, Moh. F.Kandeel, Ashraf F. El-Sherif, Ahmed S. bdel- Rahman, Synthesis, Characterization and optical properties of new Organic-Inorganic Hybrid Perovskites $[(NH_3)_2(CH_2)_3]CuCl_4$ and $[(NH_3)_2(CH_2)_4]CuCl_2Br_2$, 218 (12) 2021 Physica Status Solidi (A)
- 4-Seham K. Abdel-Aal, et al, Crystal Structure, Vibrational Spectroscopy, and Optical Properties of 1D - Organic-Inorganic Hybrid Perovskite of $[NH_3CH_2CH(NH_3)CH_2]BiCl_5$, Acta Cryst. B75, (2019)
- 5-Seham K. Abdel-Aal, Ahmed S. Abdel-Rahman, "Fascinating Physical Properties of 2D Hybrid Perovskite $[(NH_3)(CH_2)_7(NH_3)]CuCl_xBr_{4-x}$, $x = 0, 2$ and 4 " Journal of electronic materials, 48(3) (2019) 1686-1693,
- 6-Mohga Farid Mostafa, Shimaa Said El-khiyami, Seham K. Abdel-Aal, Structure, thermal, and impedance study of a new organic-inorganic hybrid $[(CH_2)_7(NH_3)_2]CoCl_4$, Journal of Physics and Chemistry of Solids, (2018), (DOI: 10.1016/j.jpcs.2018.02.048
- 7-Seham K. Abdel-Aal, Ahmed S. Abdel-Rahman, Gudrun Kocher-Oberlehner, Andrey Ionov, R.N. Mozhchil, "Structure, optical studies of two-dimensional hybrid perovskite for photovoltaic applications" Acta Cryst, A73, (2017), C1116.
- 8-Seham K. Abdel-Aal, Ahmed S. Abdel-Rahman, "Synthesis, structure, lattice energy and enthalpy of 2D perovskite hybrid $[NH_3(CH_2)_4NH_3]CoCl_4$, compared to $[NH_3(CH_2)_nNH_3]CoCl_4$, $n = 3 - 9$, J. Cryst. Growth. 457 (2017) P 282-288.
- 9-Mohga Farid Mostafa, Shimaa Said El-khiyami, Seham Kamal Abdel-Aal, Crystal structure, phase transition and conductivity study of two new organic-inorganic hybrids: $[(CH_2)_7(NH_3)_2]X_2$, $X = Cl/Br$, Journal of Molecular Structure 1127 (2017) P 59-73.