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### Computer Predictions on Hybrid Organic-Inorganic Perovskites

Hybrid or metal organic framework (MOF) perovskites of general composition,  $ABX_3$ , are known to show interesting properties which can lead to a variety of technological applications. Our first principles study shows they are also potential candidates for exhibiting cooperative spin-state transitions upon application of external stimuli,[1] and two-dimensional magnetism.[2,3] We also predict new hybrid double perovskites with B-site cation ordering. [4]

[1] *Hrishit Banerjee, Sudip Chakraborty, and Tanusri Saha-Dasgupta, Chem. Mater. 28, 8379 (2016).*

[2] *Dhani Nafday, Dipayan Sen, Nitin Kaushal, Anamitra Mukherjee, and Tanusri Saha-Dasgupta, Phys. Rev. Research 1, 032034(R) (2019).*

[3] *Dipayan Sen, Gour Jana, Nitin Kaushal, Anamitra Mukherjee, and Tanusri Saha-Dasgupta, Phys. Rev. B 102, 054411 (2020).*

[4] *Dipayan Sen, Tanusri Saha-Dasgupta and A. Cheetham, unpublished.*

Work done in collaboration with Hrishit Banerjee, Sudip Chakraborty, Dhani Nafday, Anamitra Mukherjee and Dipayan Sen.

**Saha-Dasgupta** works in the area of computational condensed matter physics/materials science. She obtained her PhD degree from Calcutta University in 1995. She was a Post-doctoral Fellow/visiting scientist in ONERA, Paris; CNRS, Cergy-Pontoise, France; Max-Planck Institute, Stuttgart, Germany and IISc, Bangalore. Saha-Dasgupta joined S.N.Bose National Centre as a lecturer in 2000. She is currently Senior Professor and Director in the same Institute. She has so far produced 14 PhD students and published more than 250 research papers. She is a fellow of American Physical Society, The World Academy of Sciences, Indian National Academy of Sciences, Indian Academy of Sciences, National Academy of Sciences, India, and West Bengal Academy of Sciences. She is recipient of Swarnajayanti Fellowship, MRSI-ICSC Superconductivity & Materials Science Annual Prize, DAE-Raja Ramanna prize, P. Sheel Memorial Award, Dr. A. P. J. Kalam HPC award and J. C. Bose National fellowship. She headed the Max-Planck-India partner group, Advanced Materials Research Unit and Thematic Unit of Excellence on Computational Materials Science at S.N.Bose National Centre.