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The role of entropy in organic-inorganic perovskites and related coordination networks

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Over the past decades, crystalline organic-inorganic network materials such as hybrid inorganic-organic perovskites (HOIPs) and metal-organic frameworks (MOFs) have changed our perception of the solid state. Such materials bring many opportunities in application-oriented research areas such as optoelectronics, photovoltaics, catalysis and gas sensing among others. At the same time, the large amount of relatively weak molecular interactions such as hydrogen bonds and dispersion interactions make materials design a challenging task. This becomes even more challenging when interested in understanding phase transitions in such materials as a function of temperature and pressure that are related to structural flexibility as observed in flexible MOFs or for ferroelectric phase transitions in HOIPs. Relatively low densities in inorganic-organic network materials facilitate the role of lattice entropy – a parameter that is barely discussed in traditional rigid-body guidelines of organic-inorganic network materials.[1,2]

In my presentation I address the role of entropic contributions in organic-inorganic coordination networks. I draw on topical examples where state-of-the-art synchrotron methods such as variable temperature high-resolution powder X-ray diffraction and Neutron Inelastic Scattering have been used to insight the thermodynamics of organic-inorganic materials. For instance, the phase evolution as function of temperature in $[\text{CH}_3\text{NH}_3]\text{PbBr}_3$ is discussed, identifying configurational entropy, lattice entropy and hydrogen bonding interactions as the critical parameters. Similar conclusions can be drawn for flexible MOFs such as ZIF-4 and $[\text{M}_2(\text{bdc})_2(\text{dabco})]$ with $\text{M} = \text{Cu}^{2+}$ and Zn^{2+} in which the balance of dispersion interactions and lattice entropy determines the underlying thermodynamics of these exciting materials.

[1] G. Kieslich, A. Goodwin, *Mater. Horiz.* 2017, 4, 362.

[2] G. Kieslich, S. Kumagai, K. T. Butler, T. Okamura, C. H. Hendon, S. Sun, M. Yamashita, A. Walsh, A. K. Cheetham, *Chem. Commun.* 2015, 51, 15538.

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