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Sub-nano cluster materials: motors, catalysts, and more



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# Sub-nano cluster materials: motors, catalysts, and more

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**Abstract:** Small clusters of main group elements and transition metals represent one of the last frontiers of inorganic chemistry. Their stabilities, shapes, and properties are often remarkable, but depend counter-intuitively and nonlinearly on cluster size and composition, to the point that any exploitation of them in applications requires serendipitous brute-force searches for suitable clusters. In this talk, we will use the qualitative language of chemical bonding, with new developments specific to clusters, as a theoretical tool of rational cluster design. We will address calculations of selected clusters, in conjunction with related spectroscopic experiments, both in the gas phase and supported on surfaces of oxides. New concepts of chemical bonding in clusters will be introduced, and we will demonstrate their utility as knobs for the design of clusters with desired shapes and functionalities, including cluster wheels, photo-driven molecular motors, and catalysts. Finally, we will touch upon our recently developed tool for modeling explicit solvent at heterogeneous interfaces at experimentally relevant temperatures and pressures.

