

Cation and Charge Ordering in Perovskite-Related Structures

Peter D. Battle

Inorganic Chemistry Laboratory, Oxford University

Keywords: perovskite, cation ordering, charge ordering

The perovskite structure possesses a high degree of compositional flexibility, being able to tolerate a wide variety of cations on both the A and B sites. Variations in the relative size and charge of the A and B cations can be accommodated in a number of ways. Some involve distortions of the ideal cubic structure and others involve the introduction of face-sharing octahedra into the network of vertex-sharing octahedra which is found in the cubic compounds. Both the A and B sites may be occupied by more than one cation species in a particular compound. In the case of the B sites this can involve cations of more than one element, or it may involve two oxidation states of the same element. In either case, the presence of more than one species raises the issue of cation ordering, either chemical ordering or charge ordering. The properties of the compound will depend on whether or not this ordering occurs; charge ordering might only occur below room temperature and the properties will therefore change on cooling. The properties of a perovskite can also be varied by modifying the dimensionality of the structure, that is by limiting the thickness of the blocks of vertex-sharing octahedra along the z axis of the cubic crystal structure. This approach recognises that perovskite is the end member of the Ruddlesden-Popper structural family. The introduction of vacancies onto the anion sublattice is another method by which the properties can be varied. Results showing the influence of cation ordering, anion vacancies, and changes in structural dimensionality on the electronic properties of perovskites will be presented.