Structural disorder and its effects on the electrical and optical properties of perovskite materials.

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Fundamental scientific studies on perovskite materials ABO_3 have been carried out intensively now days due to their unique ferroelectric and optical properties, which are of great interest in technological applications such as capacitors, transducers, sensors, nonsvolatile random-access memory devices, among others. The modulated ferroelectric and luminescence properties of these perovskite-based materials provide for a fundamental understanding of the intrinsic optical and optoelectronic properties of these systems, suggesting therefore the possibility of their rational incorporation into functional nanoscale devices. The disordered perovskite nanopowders showed strong emission of photoluminescence, which dropped to minimal levels in the ordered nanopowders. These differences in the photoluminescence of disordered and ordered nanopowders were attributed to complex cluster vacancies. Structural defects of disordered powders, in terms of band diagram, density of states, and electronic charges, were interpreted using high-level quantum mechanical calculations in the density functional framework.