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### **Computational and experimental study of functional structural distortions in layered perovskite oxides**

Layered perovskite oxides have been extensively and intensely studied because of their diverse electronic properties including ferromagnetism, ferroelectricity and superconductivity. These properties are strongly correlated with lattice distortions such as rotations, tilting and deformation of the oxygen-coordinated octahedra encompassing the B-site cations, via a strong coupling of lattice, charge and spin degrees of freedom. Here, we report two experimental and computational studies of the structure-property relationship in layered perovskite oxides. One is inversion symmetry breaking by oxygen octahedral rotations in A-site ordered  $n=1$  Ruddresden-Popper (RP) phases  $\text{NaRTiO}_4$  (R: rare earth). Synchrotron X-ray diffraction and optical second harmonic generation studies in conjunction with density functional theory (DFT) have clearly revealed that octahedral rotations represented by  $a-b0c0/b0a-c0$  in Glazer notation lead a parent centric  $P4/nmm$  phase to an acentric  $P-421m$  phase. The other is a strain-induced metal-insulator transition in an  $n=2$  RP phase  $\text{La}_3\text{Ni}_2\text{O}_7$ . Our DFT calculations show that while the bulk ground state is metallic, moderate compressive strain can drive the ground state to an insulating state in concurrence with a breathing distortion of  $\text{NiO}_6$  octahedra. This is interpreted as a Peierls transition; a band-gap opening arises from lifting and lowering of the Ni d-eg states due to the octahedral breathing. Thus, symmetry breaking due to structural distortions could lead to emergent phenomena and functionalities.

### **Biography**

Hirofumi Akamatsu has pursued his PhD from Kyoto University and Postdoctoral studies from Pennsylvania State University and Kyoto University. He has been studying various materials ranging from oxide glasses to layered perovskite oxides experimentally and theoretically. He is an Associate Professor of Department of Applied Chemistry, Kyushu University. He has been working in Tokyo Institute of Technology as an Assistant Professor. He has published more than 40 papers in reputed physics and chemistry journals.

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