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Origin of Ferroelectricity in a Family of Polar Oxides: The Dion-Jacobson Phases NICOLE BENEDEK, The University of Texas at Austin — The discovery of octahedral rotation-induced ferroelectricity has expanded the opportunities for designing materials in which the polarization is coupled to (and therefore makes possible the electric field control of) other properties, e.g. magnetism, orbital order, metal-insulator transitions. Recent work has elucidated the microscopic mechanism of octahedral rotation-induced ferroelectricity in two families of layered perovskites: $AA'B_2O_6$ double perovskites and Ruddlesden-Popper (RP) phases. However, there are many other families of layered perovskites - are there octahedral rotation-induced polar materials among them also? We use symmetry arguments, crystal chemical models and first-principles calculations to elucidate the microscopic origin of ferroelectricity in the Dion-Jacobson (DJ) phases. Although "on paper" the phenomenology of the DJ phases appears identical to that of polar double perovskites and RP phases, the crystal chemical details regarding how the polar state emerges are different. We link trends in the magnitude of the induced polarizations to changes in structure and composition and discuss possible phase transition scenarios. Our results add surprising new richness to theories of how polar structures emerge in layered perovskites.

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