Ferroelectricity, Topological Polarization and Multiferroic Order in van der Waals Materials

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van der Waals (vdW) materials are emerging as a promising avenue for future applications in nanotechnology. In addition to their useful and tunable electronic, optical, and thermoelectric properties, vdW materials also possess intriguing polar and magnetic properties, opening up new possibilities for the creation of multifunctional nanodevices. Recent studies have illustrated the exceptional ferroelectric properties of vdW materials, outperforming state-of-the-art ferroelectric field effect transistors and paving the way for advancements in nanoelectronics [1]. Additionally, by applying techniques such as twisting or straining to form moiré superlattices, it is possible to engineer networks of polar domains [2-4] with nontrivial topological character [5,6], adding another layer of complexity and potential to these materials.

We employ first-principles methods to elucidate the polar and magnetic properties of vdW materials, which have been instrumental in the understanding of the physical origin of van der Waals ferroelectricity. We provide insights into the formation of polar domains in moiré superlattices and model their response to an electric field, in excellent agreement with experimental observations [3,4]. In addition, using first-principles calculations we discovered the topologically nontrivial nature of the moiré polar domains, forming a network of polar merons and antimerons (half-skyrmions and half-antiskyrmions) [5,6].

Furthermore, we propose a general method for engineering two-dimensional (2D) multiferroics via artificial stacking of van der Waals ferroelectrics [7]. This innovative approach opens up the possibility for the discovery of a wide variety of 2D multiferroics using first-principles methods, setting the stage for the next generation of nanoscale devices.

[1] Yasuda *et. al.*, *Science* (2021)
[2] Ko *et. al.*, *Nature Materials* (2023)
[3] Bennett & Remez, *npj 2D Materials & Applications* (2022)
[4] Bennett, *Physical Review B* (2022)
[5] Bennett *et. al.*, *Nature Communications* (2023)
[6] Bennett *et. al.*, *Physical Review Research* (2023)
[7] Bennett *et. al.*, *To Be Submitted*

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