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**Tuning Magnetism and Electronic Phase Transitions by Strain and Electric Field in Zigzag MoS2 Nanoribbons**[1] LIANGZHI KOU, Bremen center of computational materials science, Germany — Effective modulation of physical properties via external control may open various potential nanoelectronic applications of single-layer MoS2 nanoribbons (MoS2NRs). We show by first-principles calculations that the magnetic and electronic properties of zigzag MoS2NRs exhibit sensitive response to applied strain and electric field. Tensile strain in the zigzag direction produces reversible modulation of magnetic moments and electronic phase transitions among metallic, half-metallic, and semiconducting states, which stem from the energy-level shifts induced by an internal electric polarization and the competing covalent/ionic interactions. A simultaneously applied electric field further enhances or suppresses the strain-induced modulations depending on the direction of the electric field relative to the internal polarization. These findings suggest a robust and efficient approach to modulating the properties of MoS2NRs by a combination of strain engineering and electric field tuning.

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