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Polar oxide interfaces: Understanding the technology of the future using first-principles calculations

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Perovskite oxides are a class of materials that display a spectacular array of physical phenomena including magnetism, ferroelectricity, piezoelectricity, and superconductivity. Incorporating such phenomena into existing semiconductor technology is one of the grand challenges of our century. However, achieving this goal has both practical and fundamental obstacles. In this talk, two polar oxide interfaces are discussed: the interface between Si/SrTiO₃ and SrTiO₃/LaAlO₃. First-principles electronic structure calculations are used to understand the practical challenge of growing SrTiO₃ on Si, and to explain the novel, highly-mobile electron gas that forms at the interface between SrTiO₃ and LaAlO₃.