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High-Throughput Design of Two-Dimensional Electron Gas Systems Based on Perovskite Oxide Heterostructures. KESONG YANG, SAFDAR NAZIR, MAZIR BEHTASH, JIANLI CHENG, Univ of California - San Diego — The perovskite-based oxide heterointerfaces between two wide-band-gap insulators such as $LaAlO_3$ and $SrTiO_3$ are attracting increasing interests because of their novel electronic properties such as the two-dimensional electron gas (2DEG) at the interface that have potential applications in the next-generation nanoelectronic devices. In this talk, we show that a group of combinatorial descriptors such as the polar character, lattice mismatch, band gap, and the band alignment between the perovskite-oxide-based band insulators and the $SrTiO_3$ substrate, can be introduced to realize a high-throughput (HT) design of $SrTiO_3$-based 2DEG systems using perovskite-oxide-oriented quantum materials database. By using these combinatorial descriptors, we have carried out a HT screening of all the polar perovskite compounds, uncovering 42 compounds of potential interests. Our approach, by defining materials descriptors solely based on the bulk materials properties, and by relying on the perovskite-oriented quantum materials repository, opens new avenues for the discovery of perovskite-oxide-based functional interface materials in a HT fashion.

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