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A unified mechanism for 2DEG at SrTiO3/LaAlO3 interface[1] LIPING YU, ALEX ZUNGER, University of Colorado at Boulder — The origin of 2DEG appearing at the TiO_2-LaO (n-type) interface between two insulating oxides of polar $LaAlO_3$ (LAO) and nonpolar $SrTiO_3$ (STO) after some critical LAO thickness is still under hot debate. Here applying modern defect theory for bulk, interface and surface, based on DFT and HSE, we investigated the current mechanisms that focus on polar catastrophe scenario, interfacial and surface O vacancies (VO), or interfacial cation defects. We uncovered a unified mechanism that can explain not only the 2DEG at n-type interface, but also the insulating behaviour at SrO/AlO_2 (p-type) interface. Specifically, for n-type interface, we found that (i) it is the VO at LAO surface coupled with built-in electric field in LAO film that causes 2DEG and determines the critical thickness. (ii) The interfacial La-on-Sr and Ti-on-Al antisite donor defects cause interfacial mixing, but do not contribute itinerant carriers. (iii) The cation vacancies and acceptor antisite defects can trap partially the 2DEG. For p-type interface, the insulating behaviour is resulted from the spontaneous formation of the defect pair of "interfacial La-on-Sr defect and surface La vacancy defect" after a critical thickness smaller than that expected from pure polar catastrophe scenario.

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