The Synergistic Effect of Hydrogen and Strain on Electronic Properties of p-Cr_2O_3/n-Fe_2O_3 Interface

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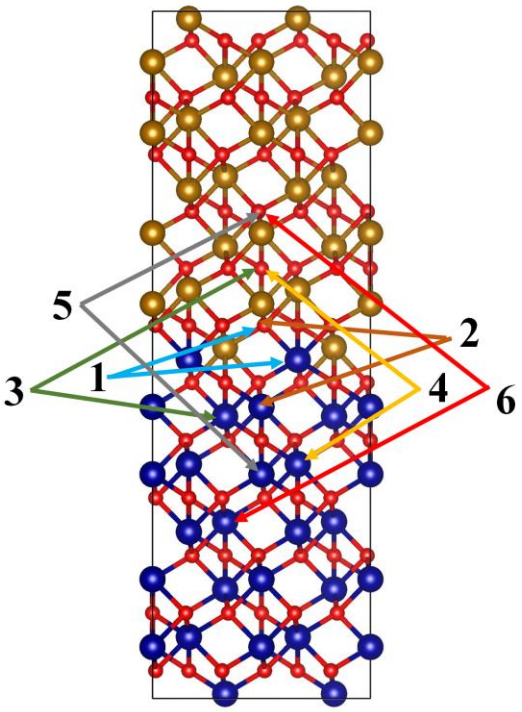
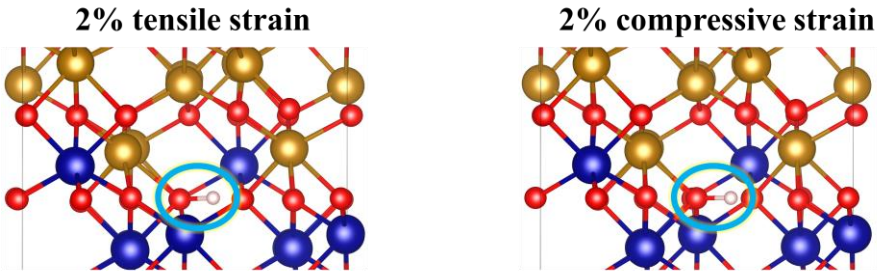


Position	Total energy (eV)
1	-1868.3168
2	-1867.7502
3	-1867.3200
4	-1867.0925
5	-1867.0567
6	-1866.9508

Figure S1. The Cr vacancy and O vacancy for interface structure in different position.

When the Cr vacancy and O vacancy are at the interface, the p-Cr_2O_3/n-Fe_2O_3 interface structure is the most stable with the lowest total energy.



	H-O bond	H charge tranfer
tensile strain	1.01 Å	0.70
compressive strain	1.03 Å	0.68

Figure S2. The structural analysis and H charge transfer under 2% tensile and compressive strain.