Tuning Energy Band-gap of Gallium Oxide Crystalline to Enhance Photoelectrochemical Water Splitting: Mixed-phase Junctions

Ming-Gang Ju[1,2], Xiang Wang[1,4], WanZhen Liang[1,3,*], Yi Zhao[1,3,*], and Can Li[1,4,*]
[1] *Collaborative Innovation Center of Chemistry for Energy Materials, Xiamen University, Xiamen 361005, China*
[2] *Department of Chemical Physics, University of Science and Technology of China, Hefei 230026, China*
[3] *State Key Laboratory of Physical Chemistry of Solid Surfaces, and Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China*
[4] *State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian National Laboratory for Clean Energy, Dalian 116023, China*
(Dated: August 5, 2014)

TABLE I: The calculated lattice constants of $\alpha-Ga_2O_3$ and $\beta-Ga_2O_3$ with the energy cutoff of 520 eV.

	$\alpha-Ga_2O_3$	$\beta-Ga_2O_3$
	Calc.	Calc.
a(Å)	5.05	12.44
b(Å)		3.08
c(Å)	13.63	5.87
γ(degree)		103.8

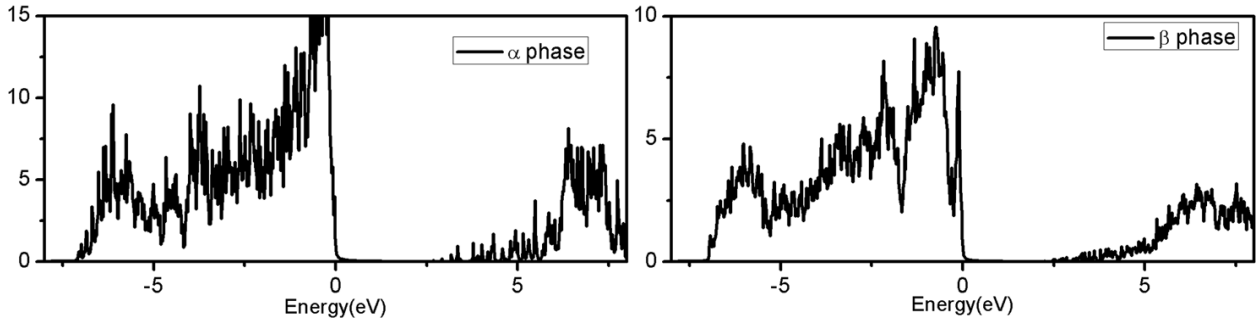

Fig. 1: The total DOS of $\alpha-Ga_2O_3$ and $\beta-Ga_2O_3$ by PBE.

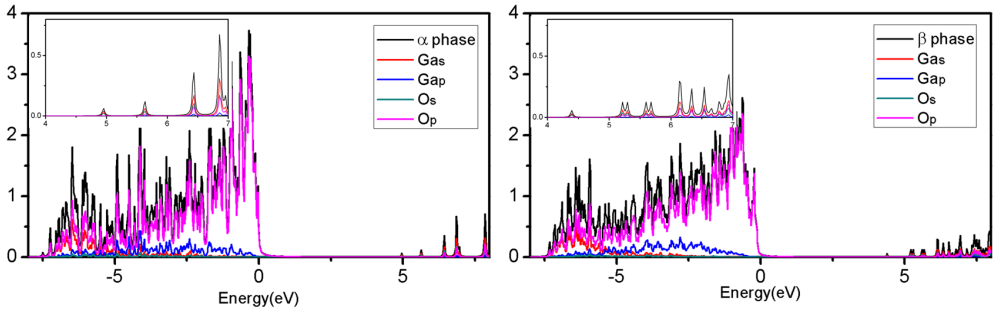

Fig. 2: The total and projected DOS of per formula unit of $\alpha-Ga_2O_3$ and $\beta-Ga_2O_3$ calculated by HSE06 functional. The conduction band are zoom in. The Fermi level is set to zero.

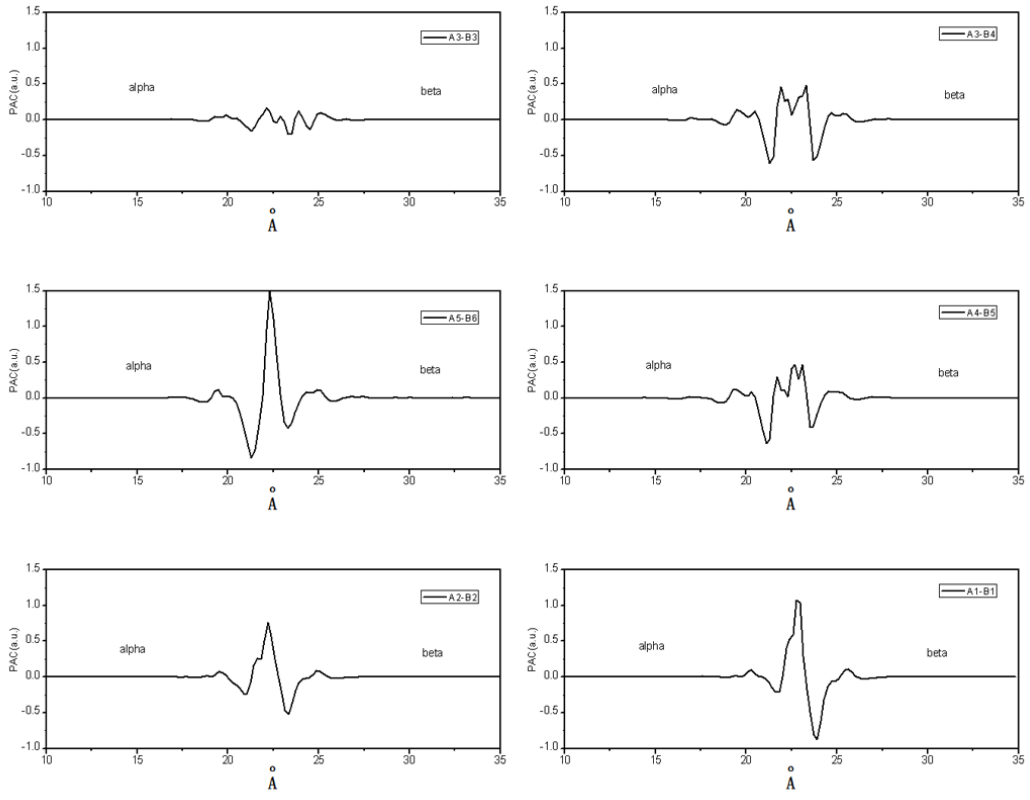

Fig. 3: The differences of PAC for the heterostructures (***b***-type) with the crystal axis angle(101°).

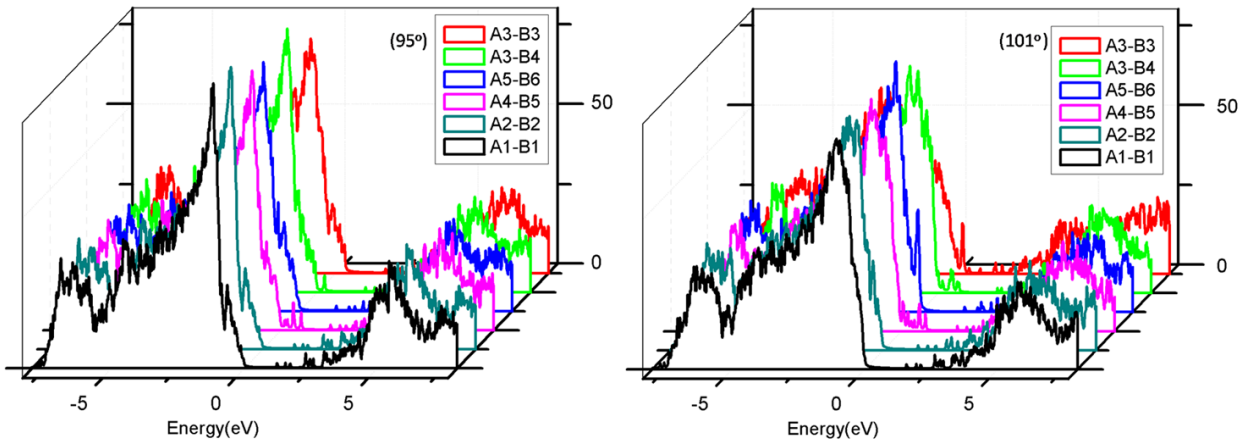

Fig. 4: The total DOS of periodic slab model of the heterostructures($\boldsymbol{a}$) with the different crystal axis angles 95°(left) and 101°(right).

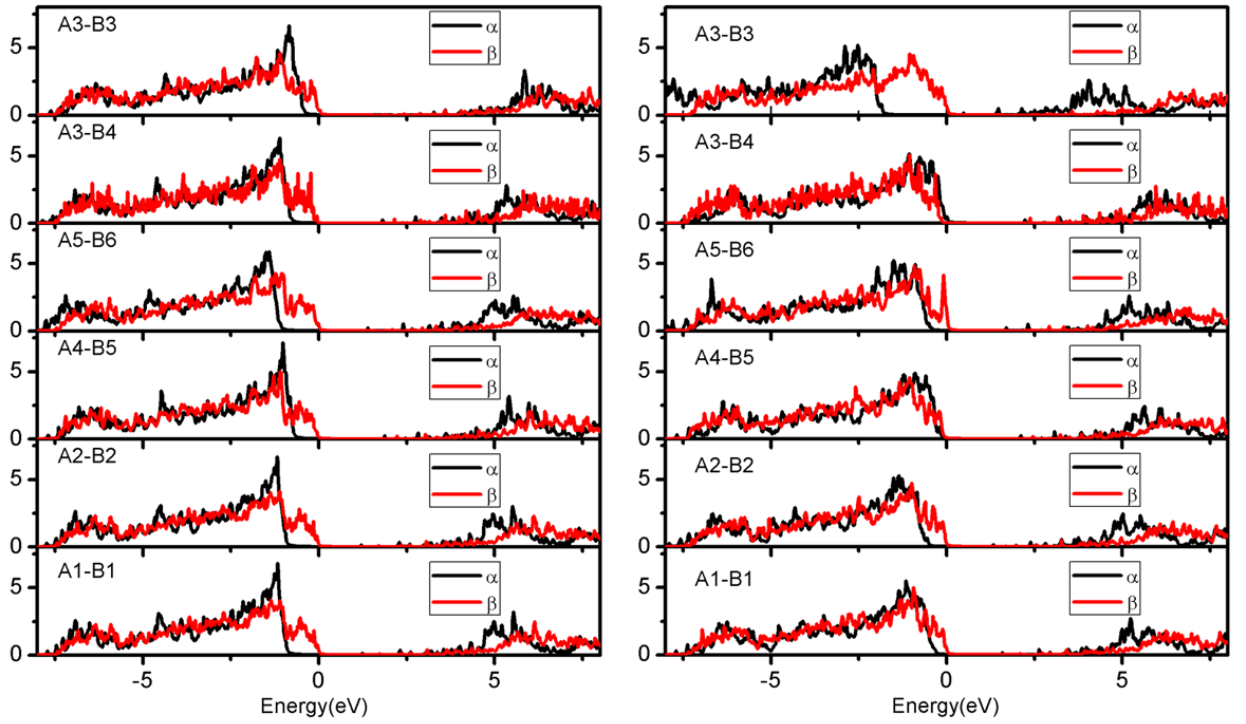

Fig. 5: The LDOS of periodic slab model of the heterostructures($\boldsymbol{a}$) with the different crystal axis angles 95°, (left) and 101°(right).

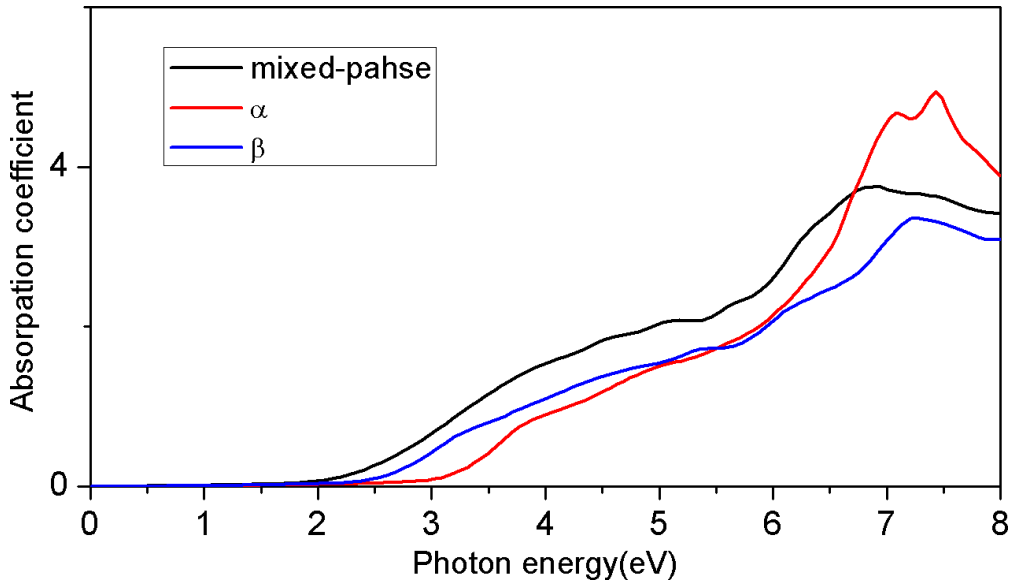

Fig. 6: The optical absorption curves of the mixed-phase and the two pure phases by PBE.

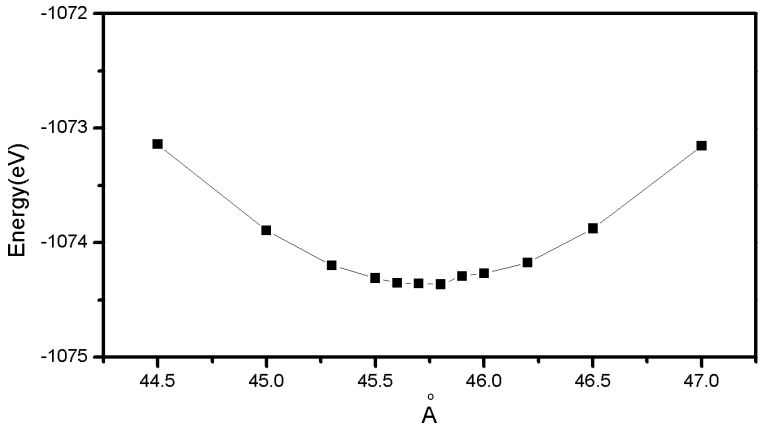

Fig. 7: The calculated energies of ***b***-type heterostructures A1-B1 with different lengths and the most stable heterostructure with length 45.8Å. ($\phi = 101^\circ$)

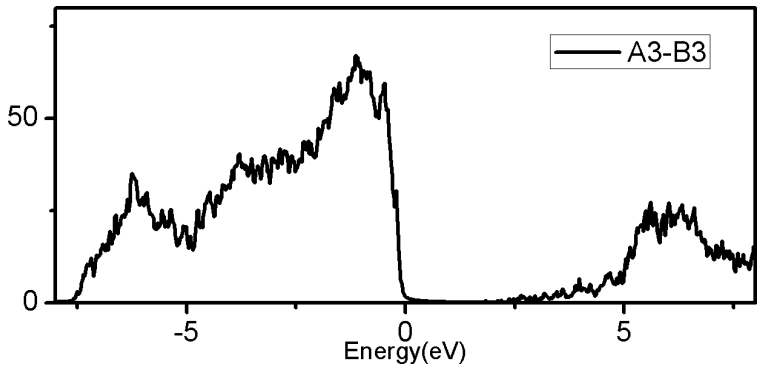

Fig. 8: The total DOS of ***b***-type heterostructures A1-B1 with length 45.8 Å.($\phi = 101^\circ$)

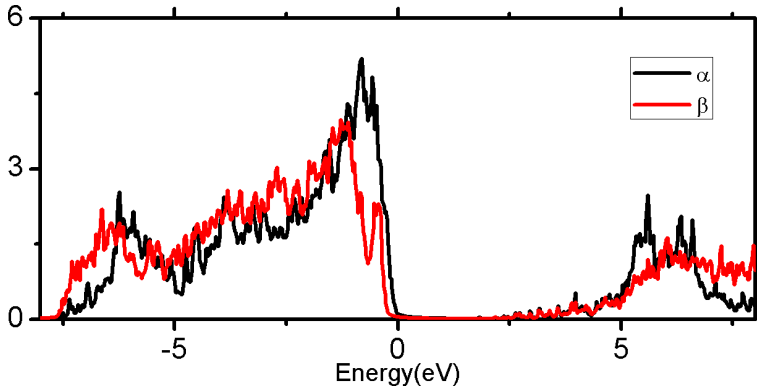

Fig. 9: The LDOSs of ***b***-type heterostructures A1-B1 with length 45.8 Å.($\phi = 101°$)

* Electronic address: liangwz@xmu.edu.cn,yizhao@xmu.edu.cn,canli@dicp.ac.cn