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## Supplementary Material

2 Insight into the interface engineering between methylammonium lead halide  
3 perovskite and gallium oxide: a first-principles approach

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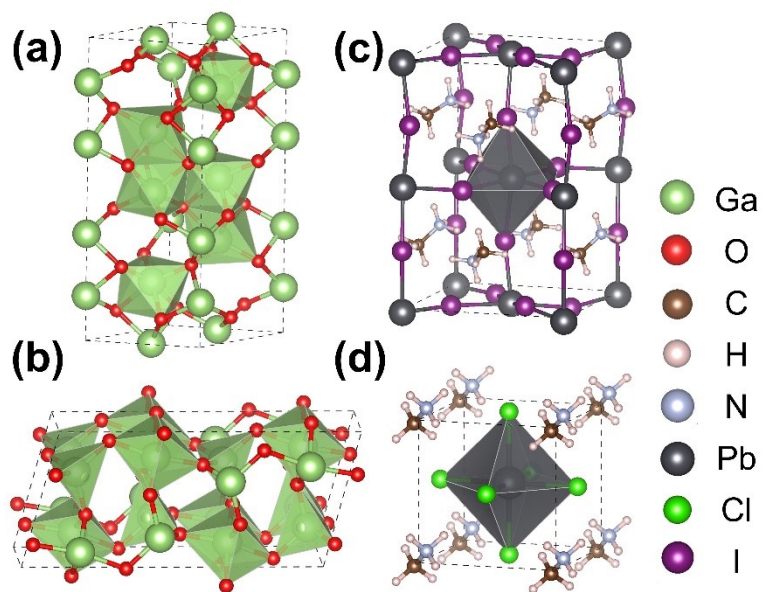
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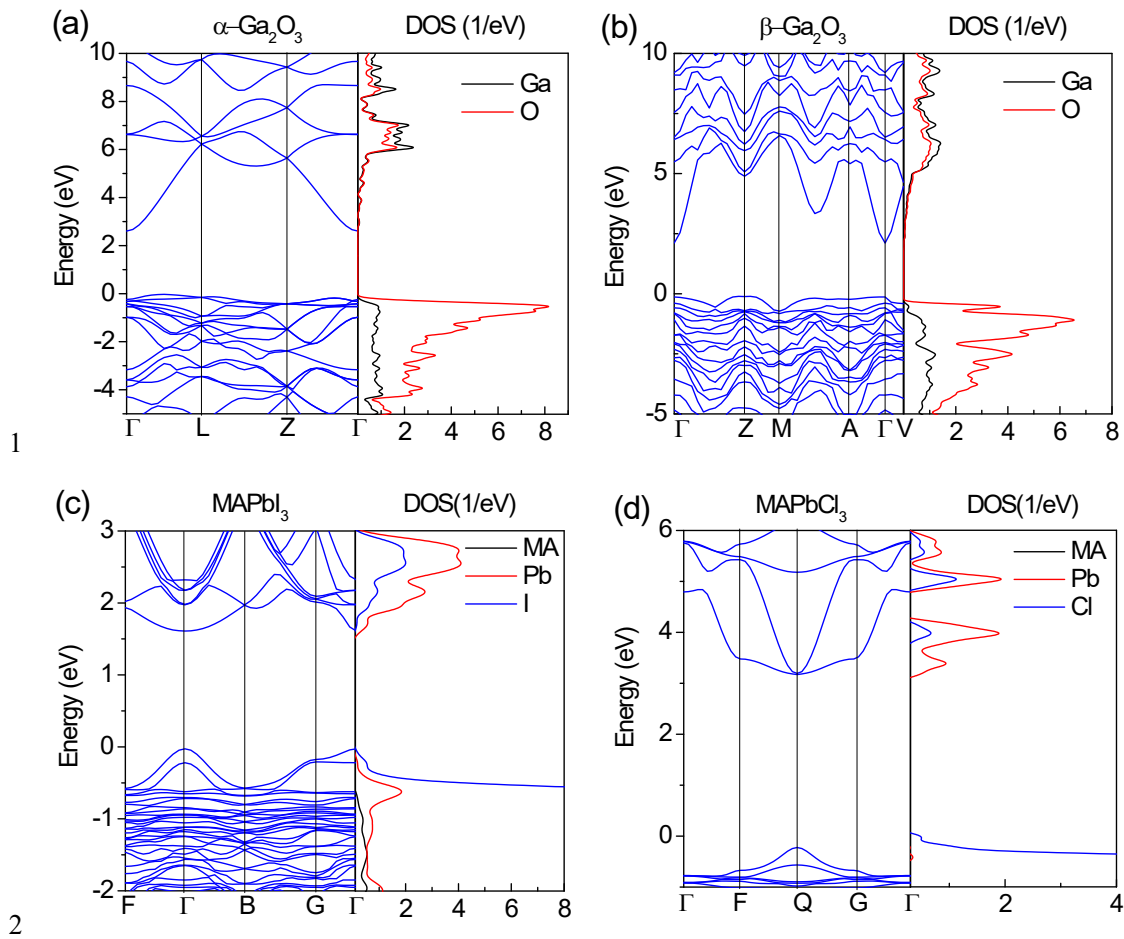
13 *E-mail:* [guoyao@ayit.edu.cn](mailto:guoyao@ayit.edu.cn) (Y. Guo), [wangyuhua@wust.edu.cn](mailto:wangyuhua@wust.edu.cn) (Y. Wang).

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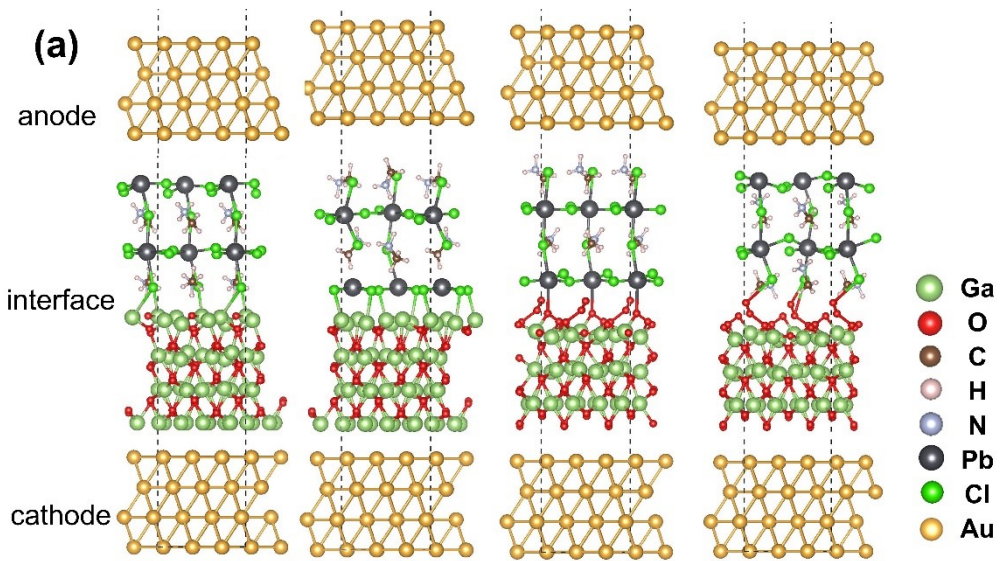


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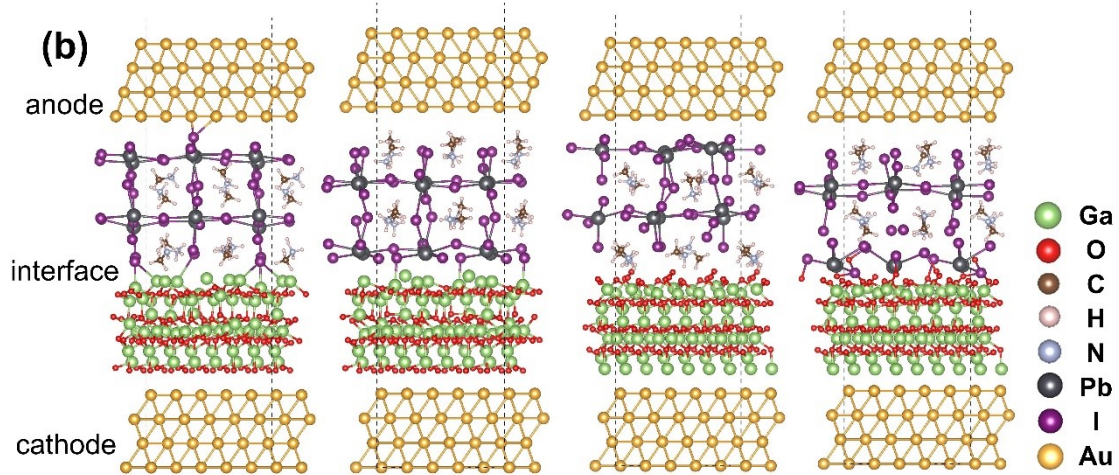
2 **Figure S1** Crystal structures of (a)  $\alpha$ - $\text{Ga}_2\text{O}_3$ , (b)  $\beta$ - $\text{Ga}_2\text{O}_3$ , (c) pseudo-tetragonal  $\text{MAPbI}_3$ ,  
 3 and (d) pseudo-cubic  $\text{MAPbCl}_3$ .



3 **Figure S2** Band structures and DOS of (a)  $\alpha$ - $\text{Ga}_2\text{O}_3$ , (b)  $\beta$ - $\text{Ga}_2\text{O}_3$ , (c) pseudo-tetragonal  
 4  $\text{MAPbI}_3$ , and (d) pseudo-cubic  $\text{MAPbCl}_3$ .



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3 **Figure S3** Device structures of the perovskite/Ga<sub>2</sub>O<sub>3</sub> interfaces (a) MAPbCl<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub>, (b)

4 MAPbI<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub>.

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- 1 **Table S1** Calculated and experimental lattice constants ( $\text{\AA}$ ) of  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub>,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>,  
 2 pseudo-tetragonal MAPbI<sub>3</sub>, and pseudo-cubic MAPbCl<sub>3</sub>.

		<i>a</i>	<i>b</i>	<i>c</i>
$\alpha$ -Ga <sub>2</sub> O <sub>3</sub>	Calc.	5.07	5.07	13.22
	Ref.	4.98	4.98	13.44
$\beta$ -Ga <sub>2</sub> O <sub>3</sub>	Calc.	12.28	3.07	5.84
	Ref.	12.22	3.04	5.81
MAPbCl <sub>3</sub>	Calc.	6.08	6.08	6.08
	Ref.	5.68	5.68	5.68
MAPbI <sub>3</sub>	Calc.	8.77	8.77	13.01
	Ref.	8.85	8.85	12.44

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1 **Table S2** Lattice parameter (Å) of the free layers and interfaces.

	<i>a</i>	<i>b</i>
$\alpha$ -Ga <sub>2</sub> O <sub>3</sub> (110)	7.33	5.29
$\beta$ -Ga <sub>2</sub> O <sub>3</sub> (-201)	7.55	3.07
MAPbCl <sub>3</sub> (100)	6.08	6.08
MAPbI <sub>3</sub> (110)	13.00	12.40
MAPbCl <sub>3</sub> /Ga <sub>2</sub> O <sub>3</sub>	8.69	8.69
MAPbI <sub>3</sub> /Ga <sub>2</sub> O <sub>3</sub>	13.02	11.39

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1 **Table S3** Lattice mismatch (%) of the perovskite/Ga<sub>2</sub>O<sub>3</sub> interfaces.

	MAPbCl <sub>3</sub> /Ga <sub>2</sub> O <sub>3</sub>	MAPbI <sub>3</sub> /Ga <sub>2</sub> O <sub>3</sub>
lattice mismatch	3.6	4.5

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