

Supporting Information for

**Ferroelastic Domains Drive Charge Separation and Suppress  
Electron–Hole Recombination in All–Inorganic Halide  
Perovskites: Time–Domain Ab Initio Analysis**

Ran Shi,<sup>1</sup> Zhaosheng Zhang,<sup>2</sup> Wei–hai Fang,<sup>1</sup> and Run Long,<sup>1\*</sup>

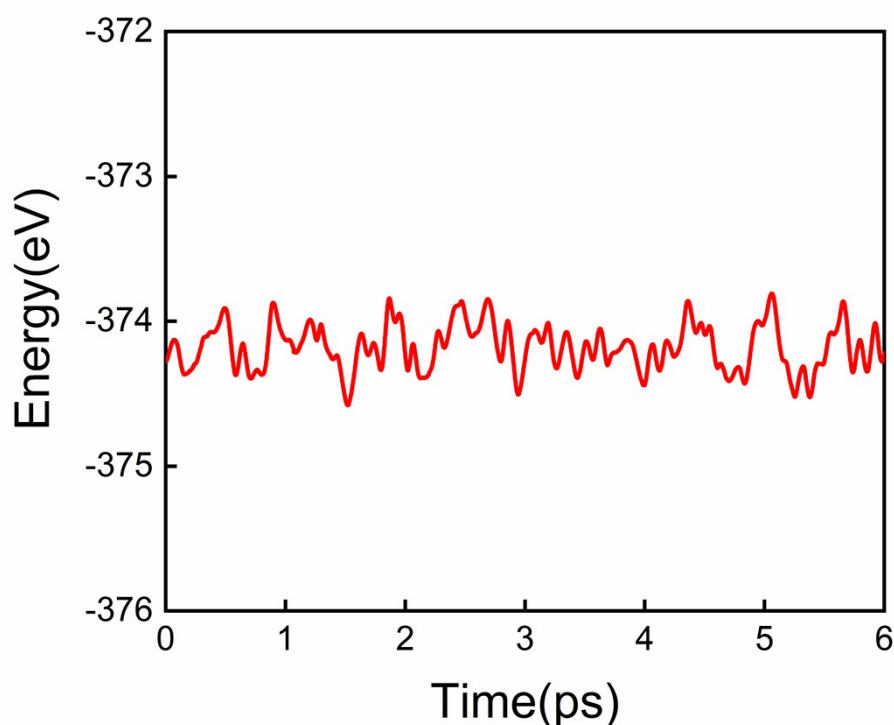
<sup>1</sup>*College of Chemistry, Key Laboratory of Theoretical & Computational*

*Photochemistry of Ministry of Education, Beijing Normal University, Beijing, 100875,*

*People's Republic of China*

<sup>2</sup>*College of Chemistry & Environmental Science, Hebei University, Baoding,*

*071002, People's Republic of China*



**Figure S1.** The evolution of total energy for the CsPbBr<sub>3</sub> containing ferroelastic domains of 6 ps MD simulation.

---

\* Corresponding Author Email: runlong@bnu.edu.cn