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Supporting Information

Understanding the sensing mechanisms of perovskite materials for gases with different properties, a perspective from the oxidation-reduction states of the central metal ions

Bing Zhang,[a,b,c] Yang Yang,[b] Lei Tong,[b] Xiaogang Wang,[b] Bin Hu,[a,b,c] Li Zhao,[a,b] Qiang Lu*[,a,b,c]

[a] National Engineering Laboratory for Biomass Power Generation Equipment, North China Electric Power University, Beijing 102206, P. R. China;

[b] School of New Energy, North China Electric Power University, Beijing 102206, P. R. China;

[c] State Key Laboratory of Alternate Electrical Power System with Renewable Energy Sources, North China Electric Power University, Beijing 102206, P. R. China.

[*] Corresponds author: Email: qlu@ncepu.edu.cn , qianglu@mail.ustc.edu.cn ; Tel.: +86 10 61771335; Fax: +86 10 61772032(801).

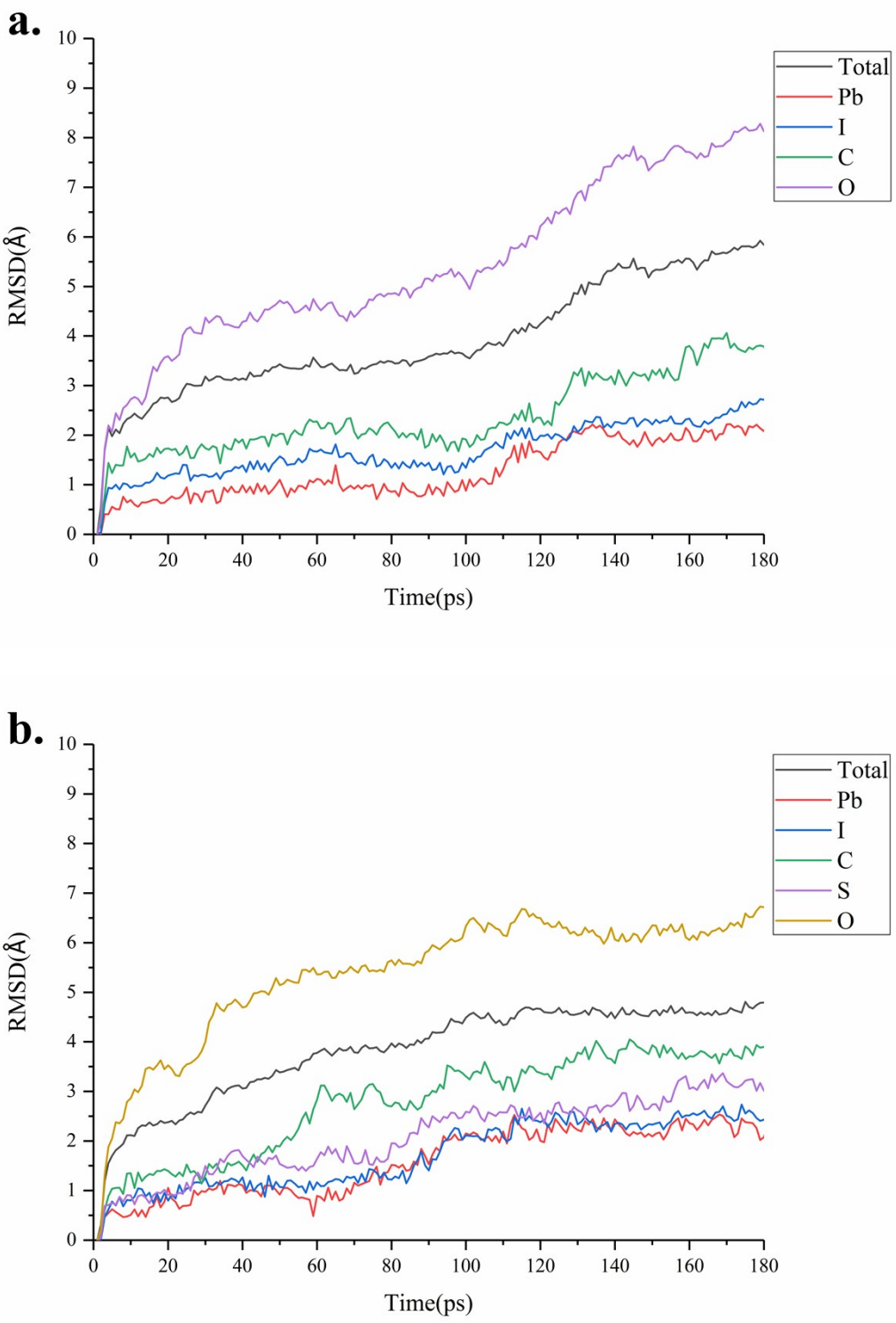
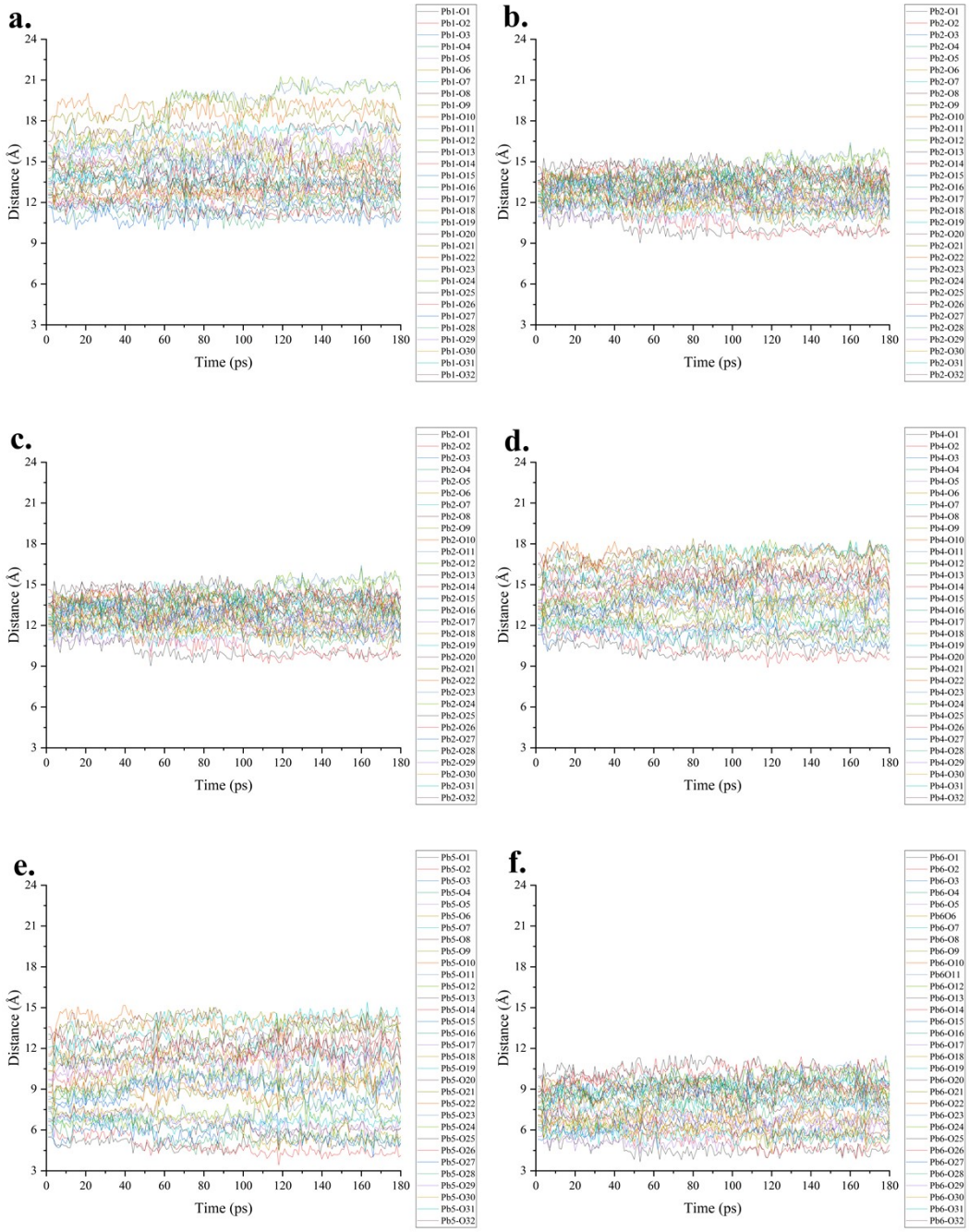


Fig. S1 The RMSD of (a) $CH_3NH_3PbI_3$, and (b) $(CH_3NH_3)_2Pb(SCN)_2I_2$.


a.
Distance (Å)
Time (ps)
Pb1-O1
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Pb1-O5
Pb1-O6
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Pb1-O8
Pb1-O9
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Pb1-O32
b.
Distance (Å)
Time (ps)
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d.
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e.
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f.
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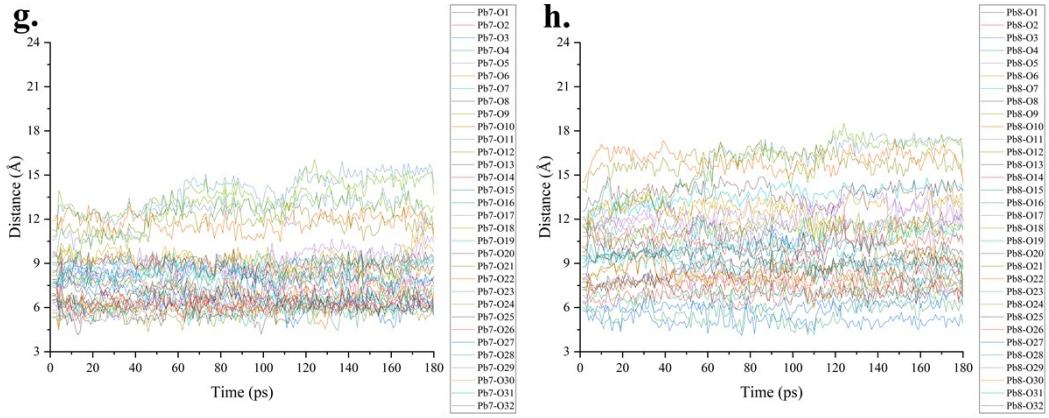

Fig. S2 The distances of (a) Pb1-O, (b) Pb2-O, (c) Pb3-O, (d) Pb4-O, (e) Pb5-O, (f) Pb6-O, (g) Pb7-O and (h) Pb8-O in $CsPbBr_3 \bullet 16O_2$ system.

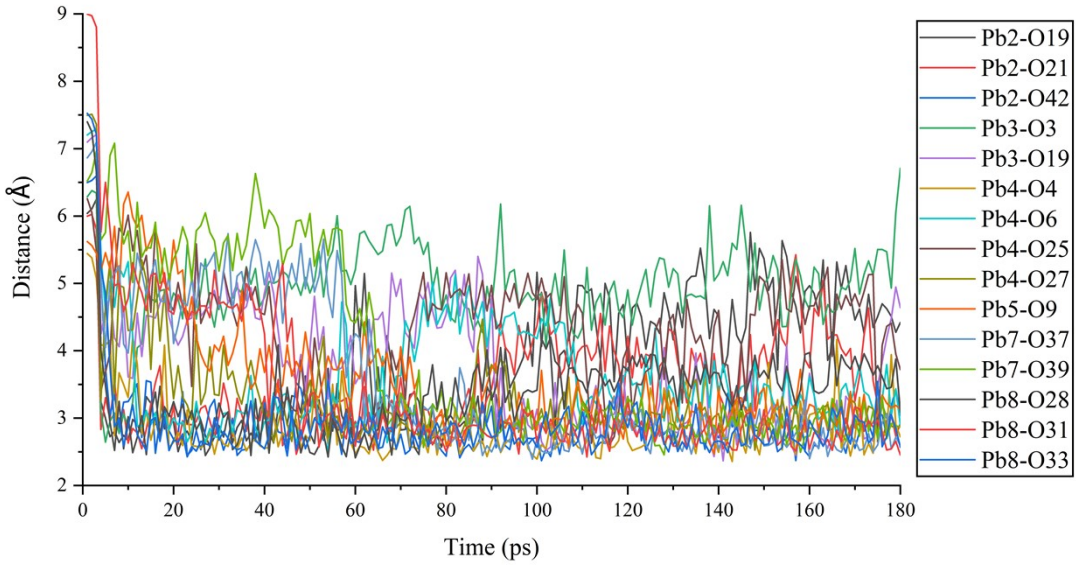

Fig. S3 The interaction fluctuations between Pb and O3 during the simulations.

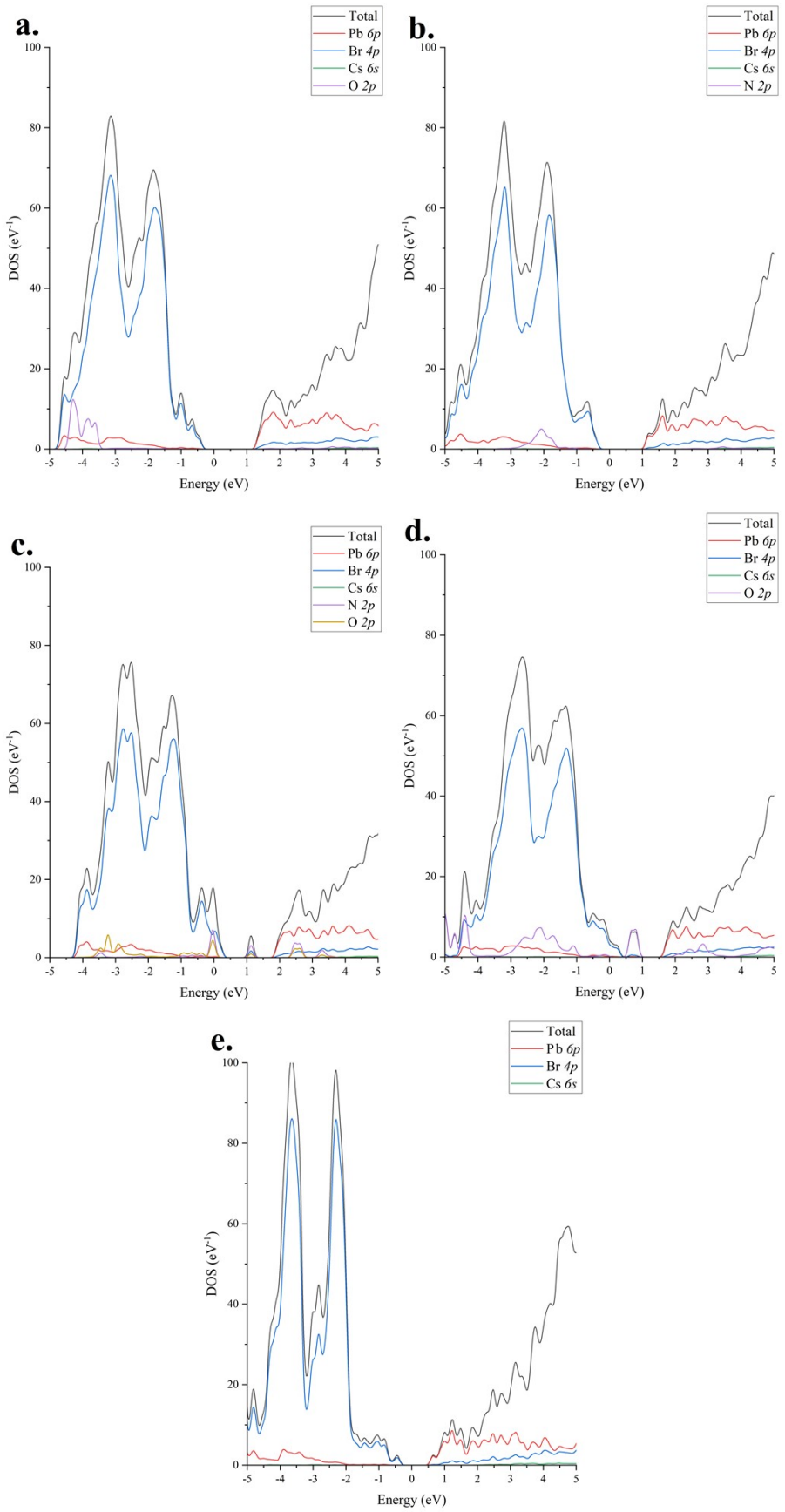

Fig. S4 The density of states (DOS) of (a) $CsPbBr_3$-H_2O, (b) $CsPbBr_3$-NH_3, (c) $CsPbBr_3$-NO_2, (d) $CsPbBr_3$-O_3 and (e) $CsPbBr_3$, respectively.