

Supporting Information File

A DFT Study of Alkaline Earth Metal-Doped FAPbI₃ (111) and (100) Surfaces

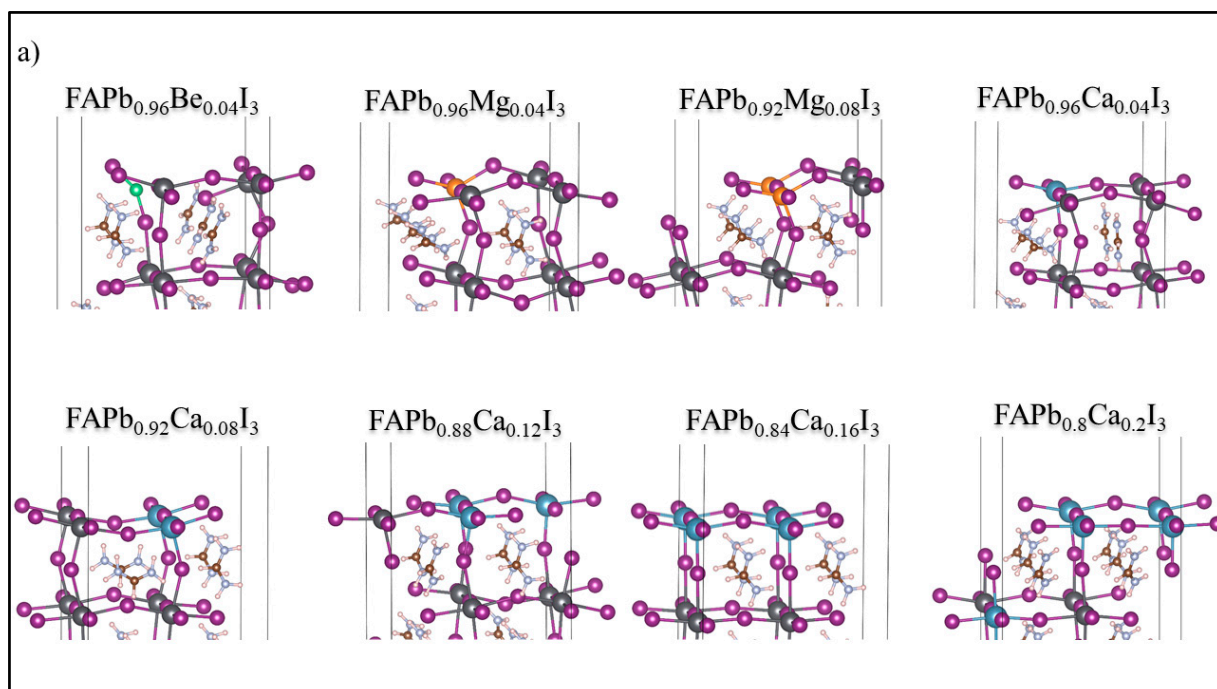
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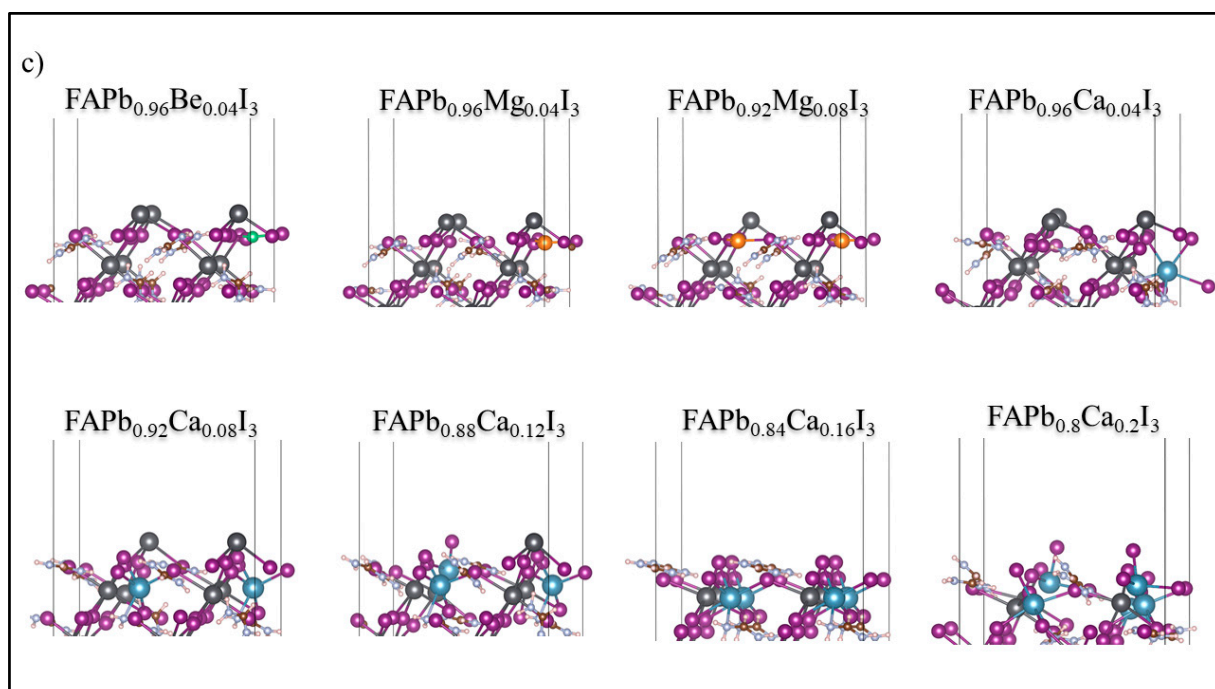
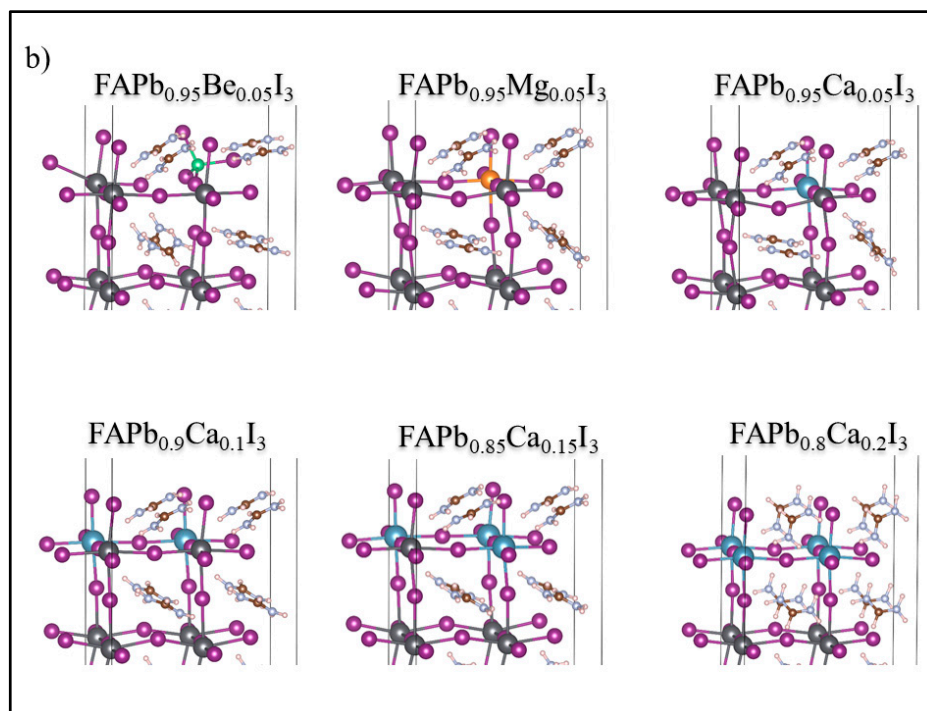
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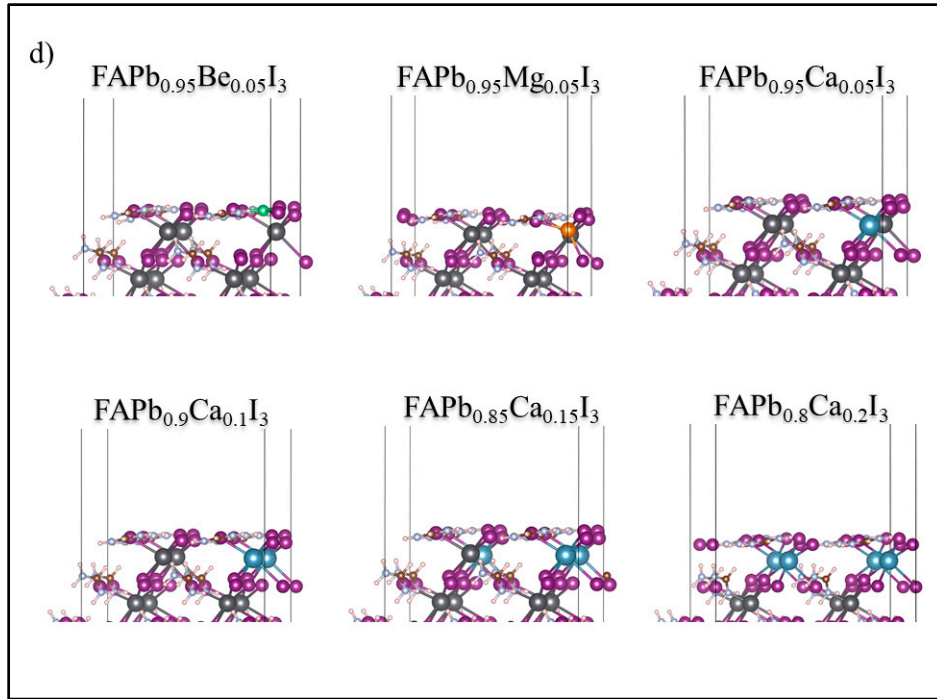
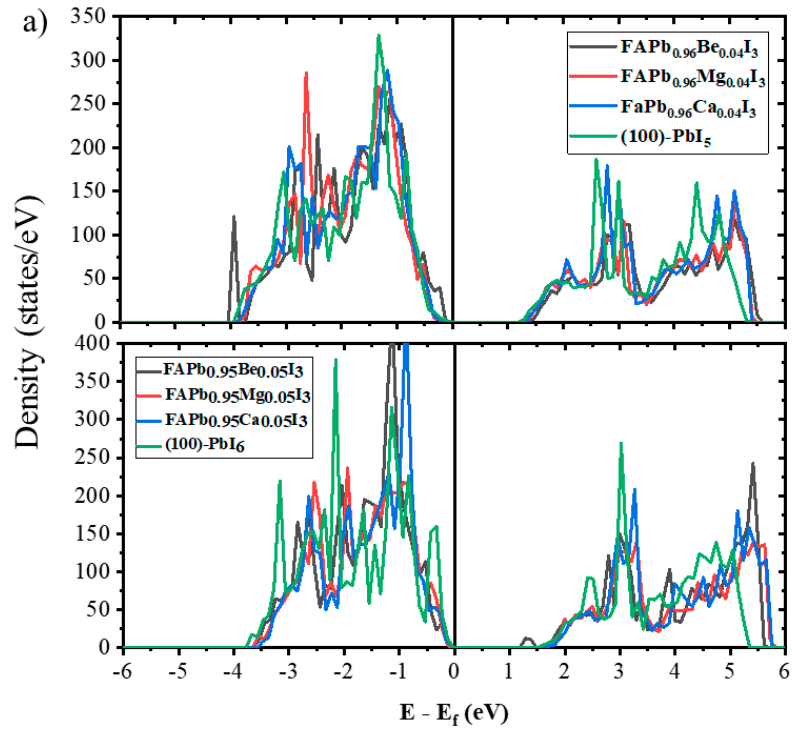


Figure S1. Three-dimensional (3D) depiction of Be (green), Mg (orange), and Ca (blue)-doped FAPI surfaces related to: a) (100)-PbI₅, b) (100)-PbI₆, c) (111)-PbI₃, and d) (111)-PbI₆ terminations.



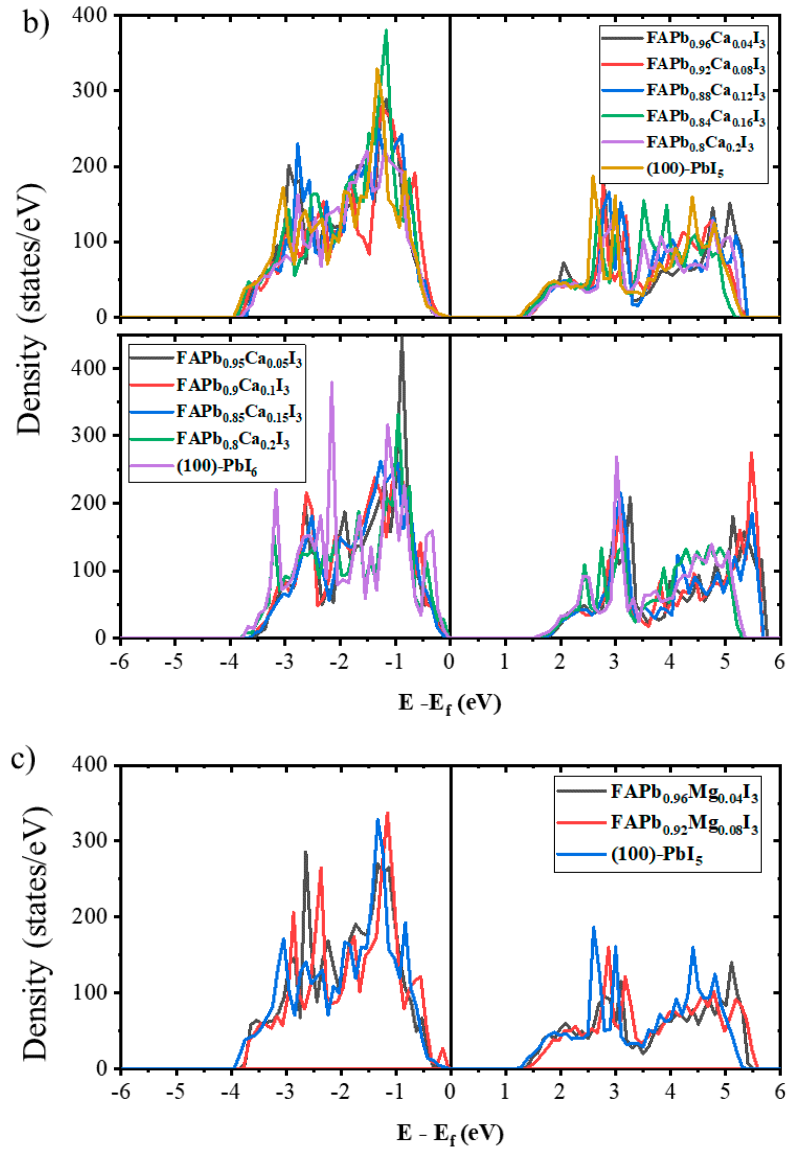
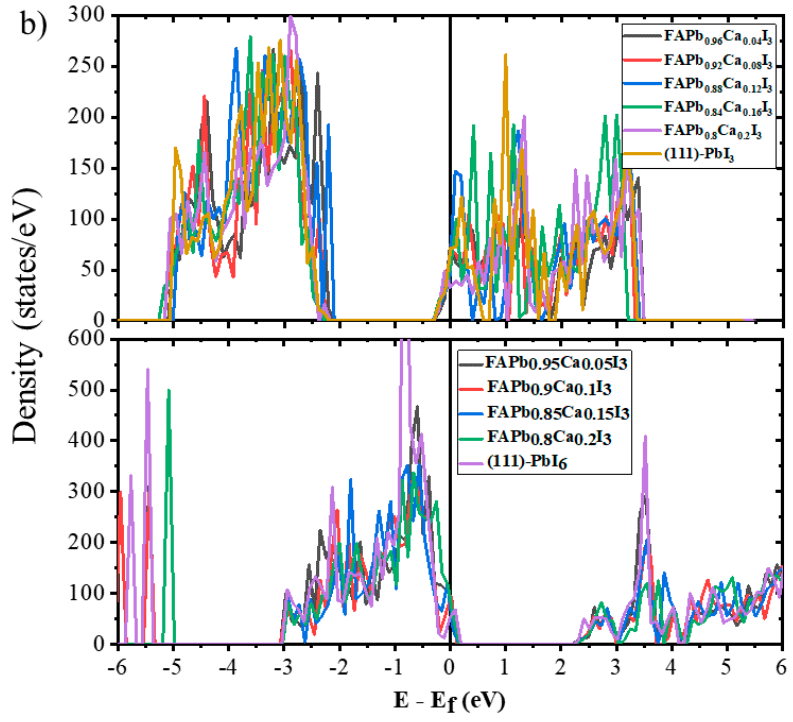
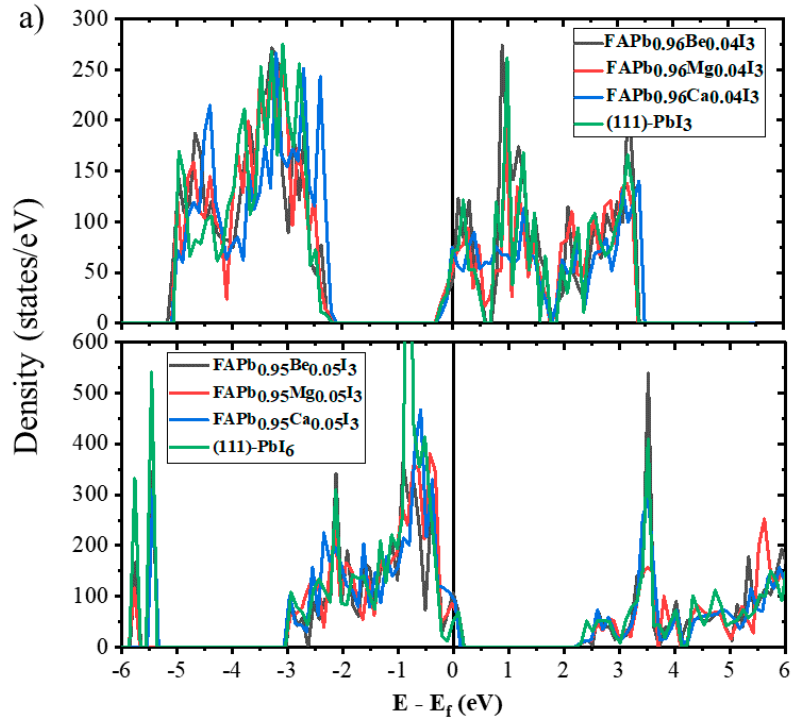


Figure S2. The total density of states for (100) surfaces with doping of a) 1 atom of Be, Mg, and Ca in PbI₅ and PbI₆ terminations, b) 1-4 atoms of Ca in PbI₆ and 1-5 atoms of Ca in PbI₅ terminations, and c) 1-2 atoms of Mg in PbI₅ termination. The Fermi level is set at zero eV.



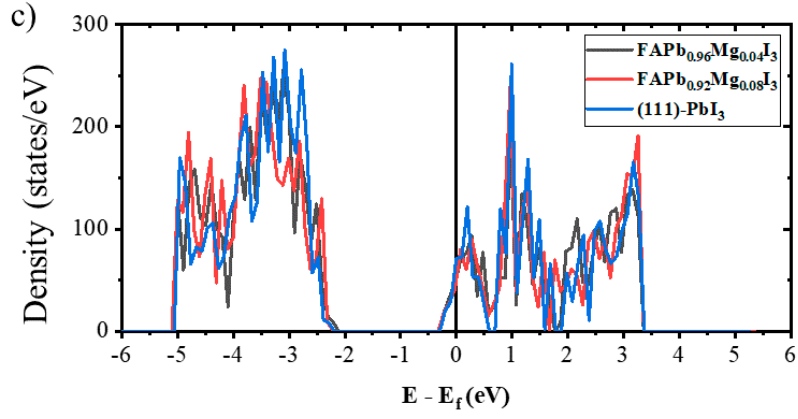
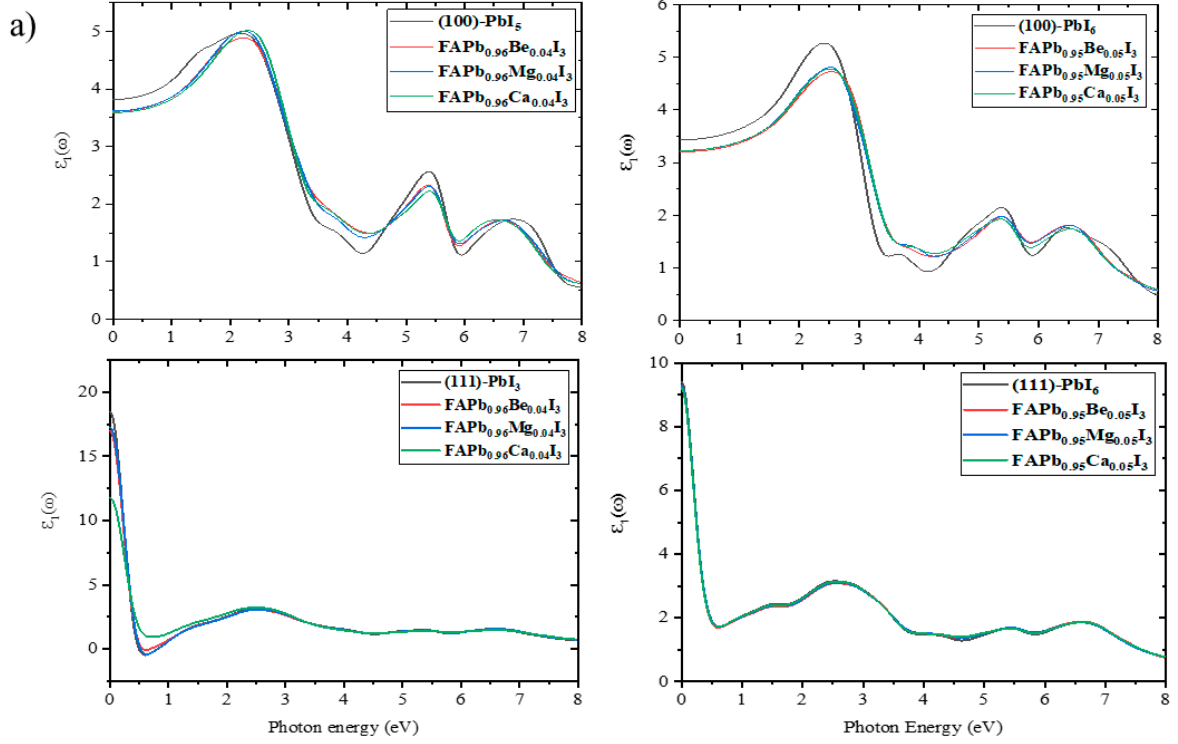


Figure S3. The total density of states for (111) surfaces with doping of a) 1 atom of Be, Mg, and Ca in PbI_3 and PbI_6 terminations, b) 1-4 atoms of Ca in PbI_6 and 1-5 atoms of Ca in PbI_3 terminations, and c) 1-2 atoms of Mg in PbI_3 termination. The Fermi level is set at zero eV.



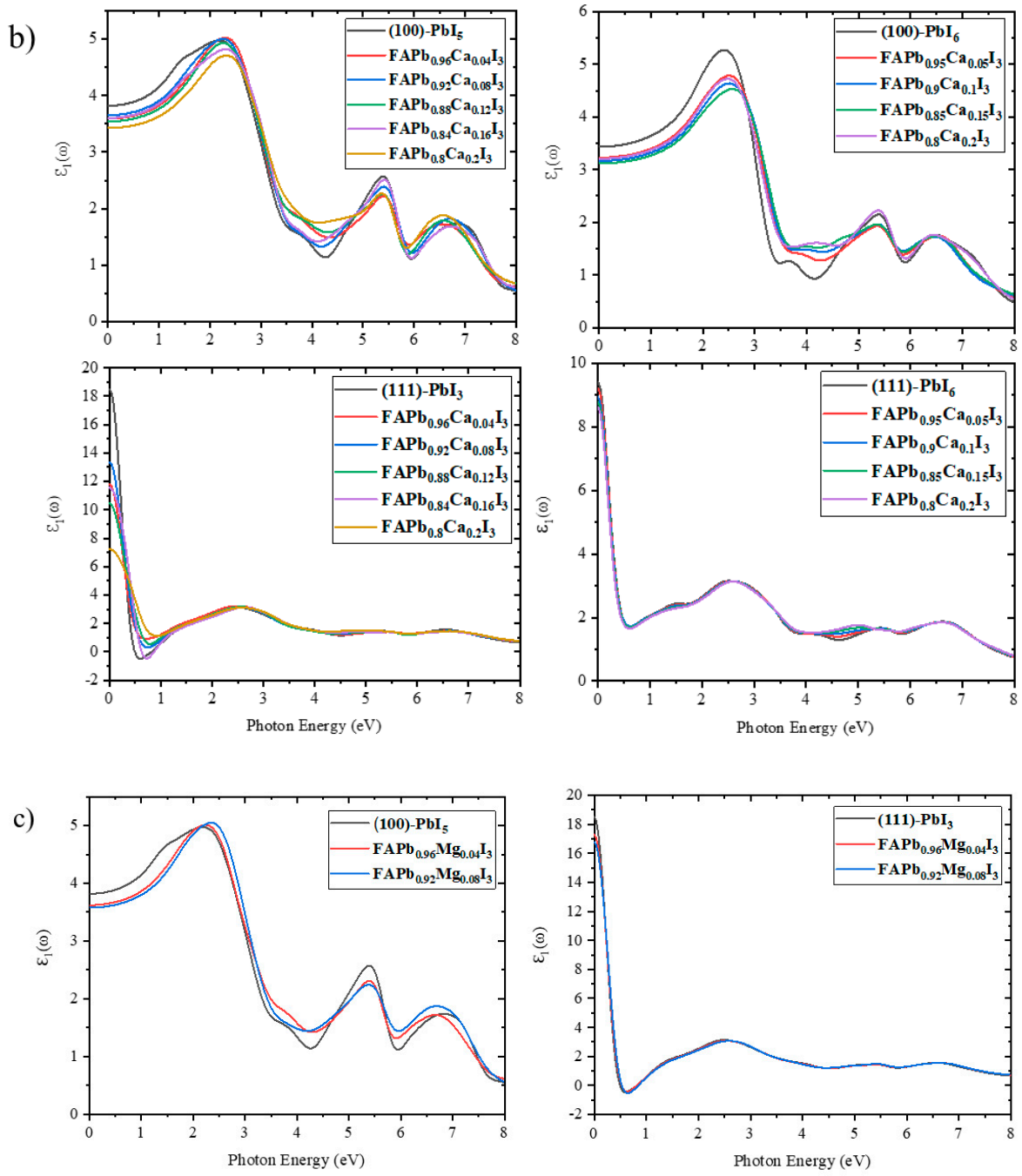
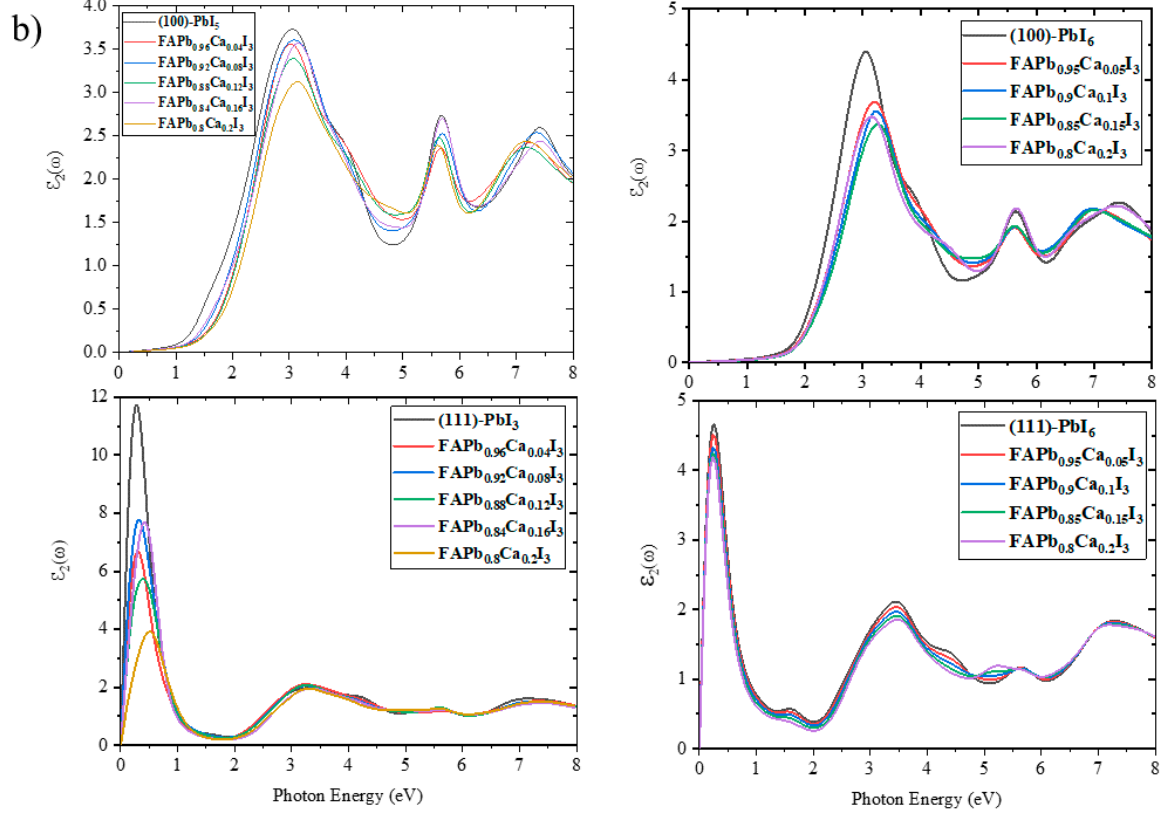
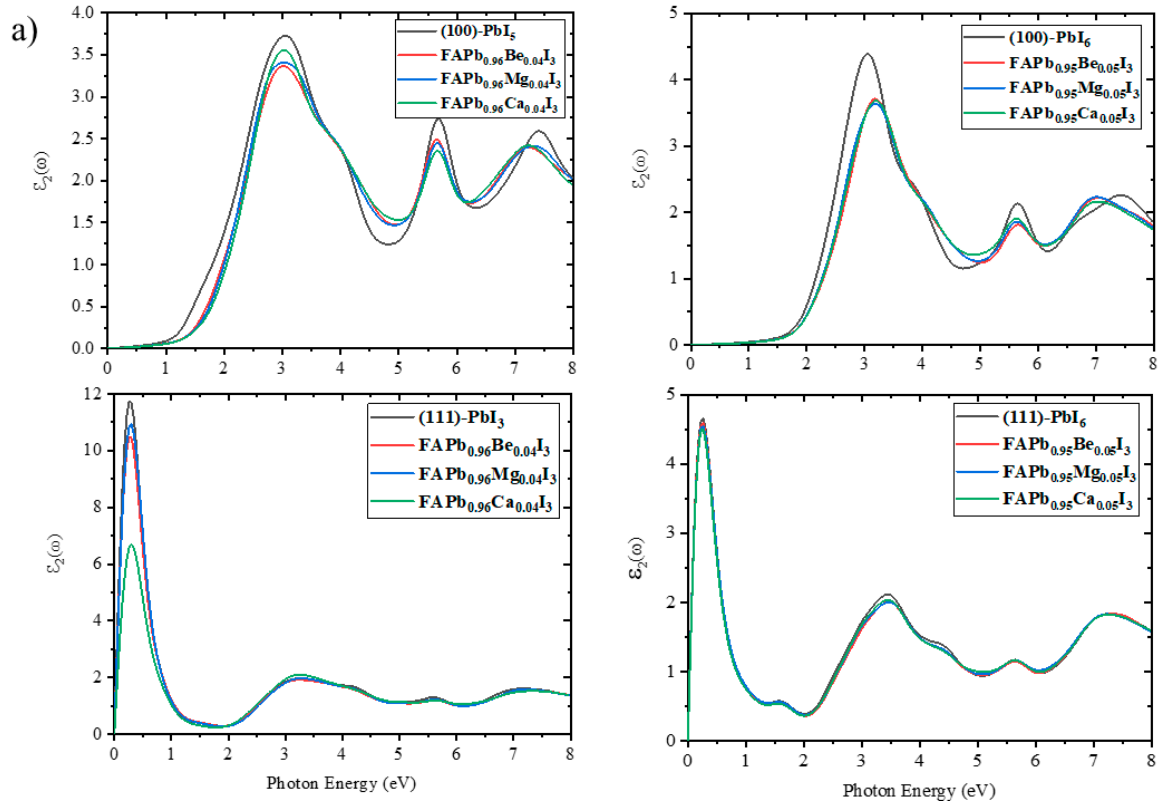


Figure S4. The real part of dielectric function for (100) and (111) surfaces with doping of a) 1 atom of Be, Mg, and Ca in all terminations, b) 1-4 atoms of Ca in both PbI₆ terminations and 1-5 atoms of Ca in PbI₅ and PbI₃ terminations, and c) 1-2 atoms of Mg in PbI₃ and PbI₅ terminations.



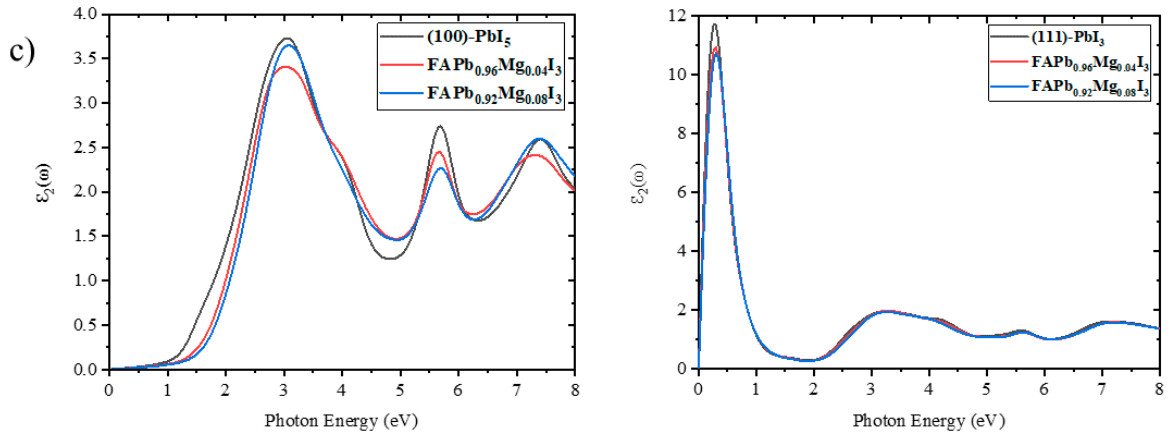
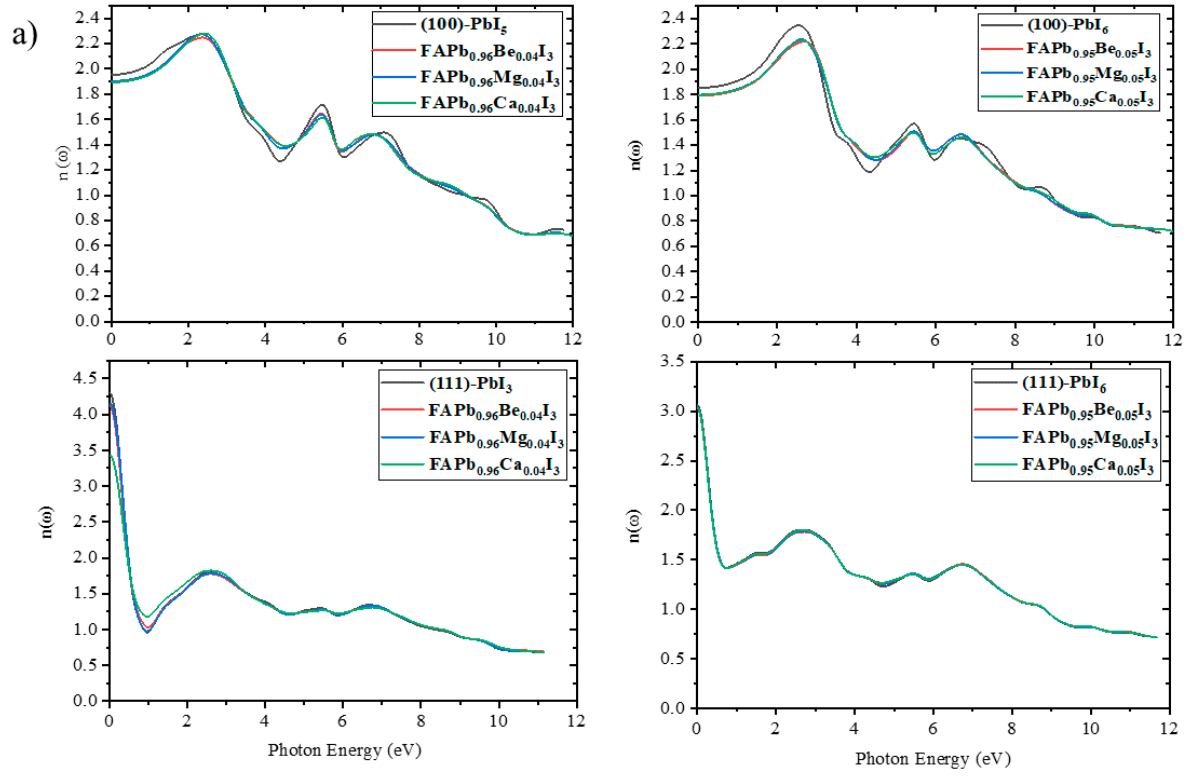


Figure S5. The imaginary part of dielectric function for (100) and (111) surfaces with doping of a) 1 atom of Be, Mg, and Ca in all terminations, b) 1-4 atoms of Ca in both PbI₆ terminations and 1-5 atoms of Ca in PbI₃ and PbI₅ terminations, and c) 1-2 atoms of Mg in PbI₃ and PbI₅ terminations.



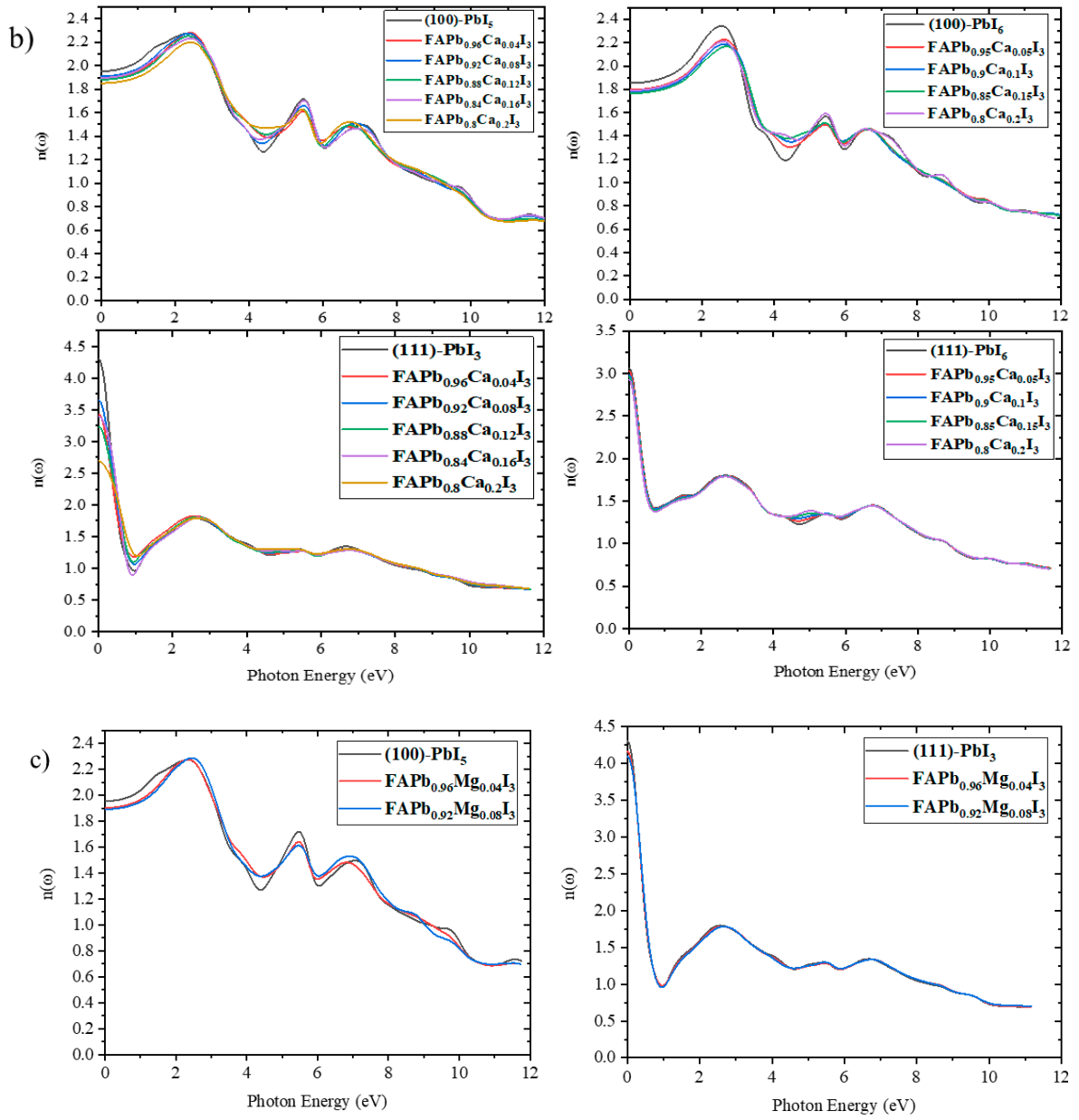
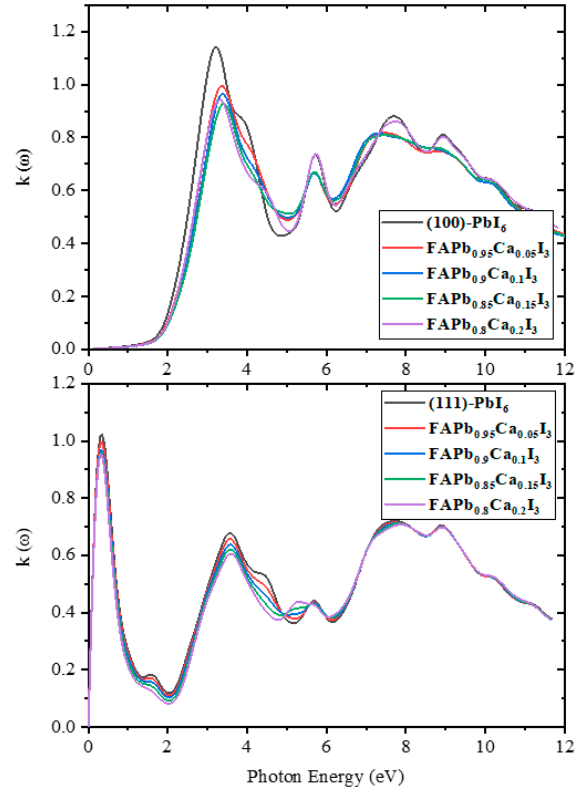
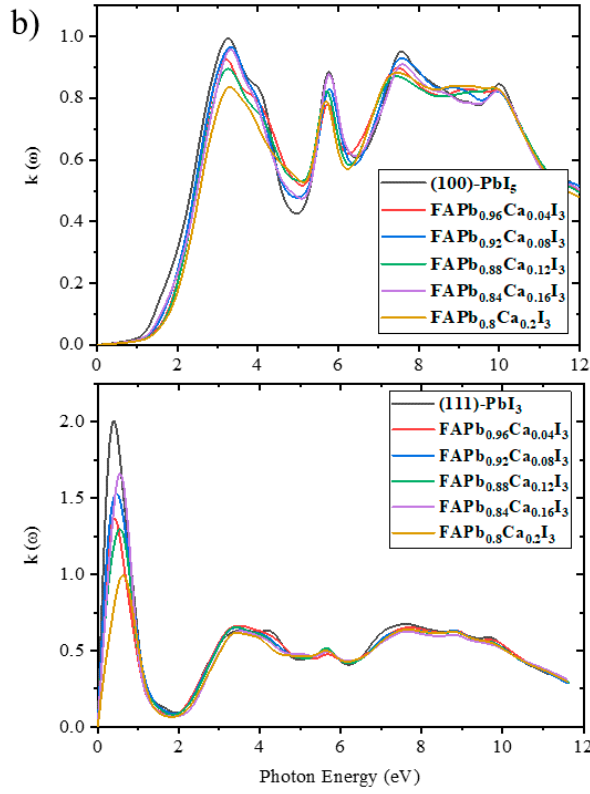
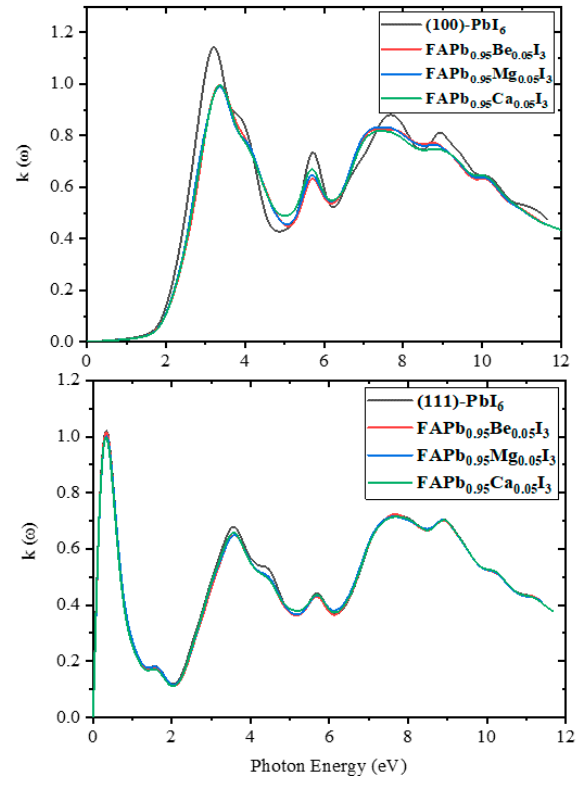
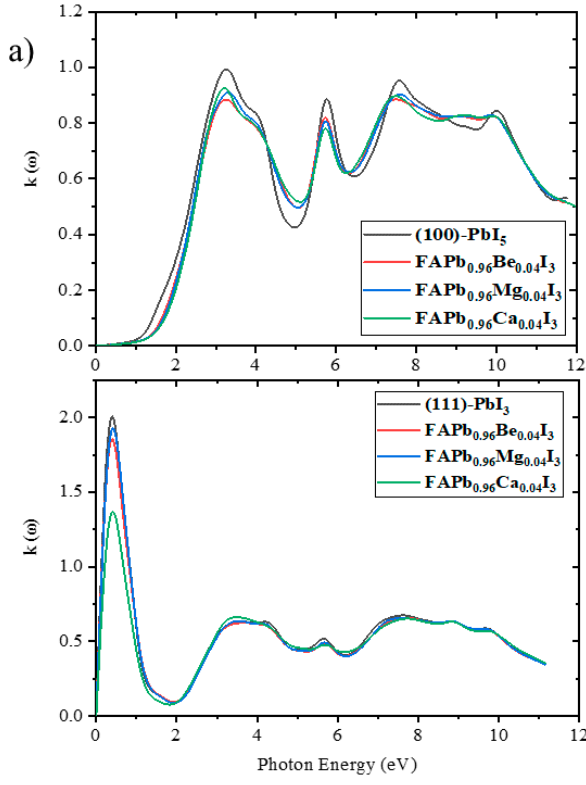


Figure S6. The refractive index spectra for for (100) and (111) surfaces with doping of a) 1 atom of Be, Mg, and Ca in all terminations, b) 1-4 atoms of Ca in both PbI_5 terminations and 1-5 atoms of Ca in PbI_5 and PbI_3 terminations, and c) 1-2 atoms of Mg in PbI_3 and PbI_5 terminations.



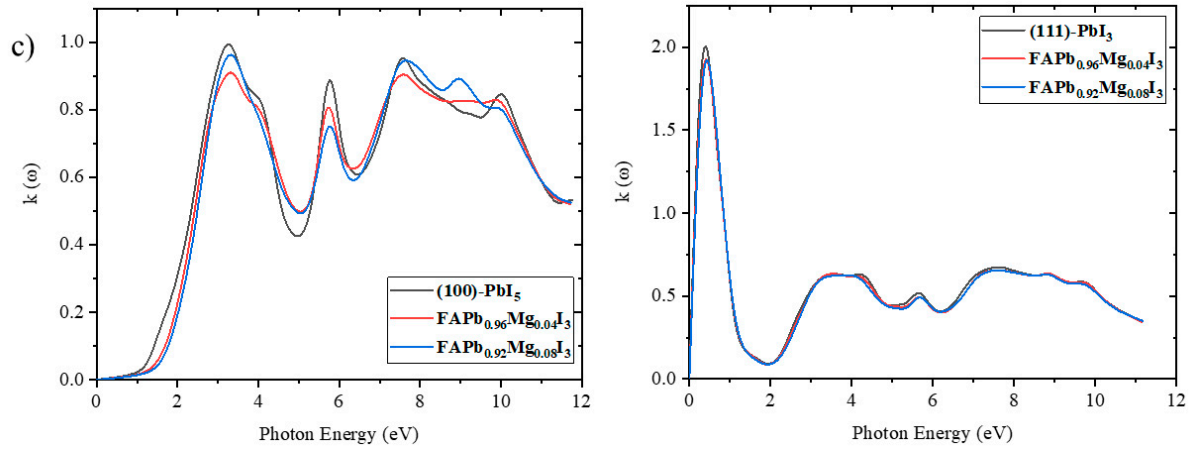
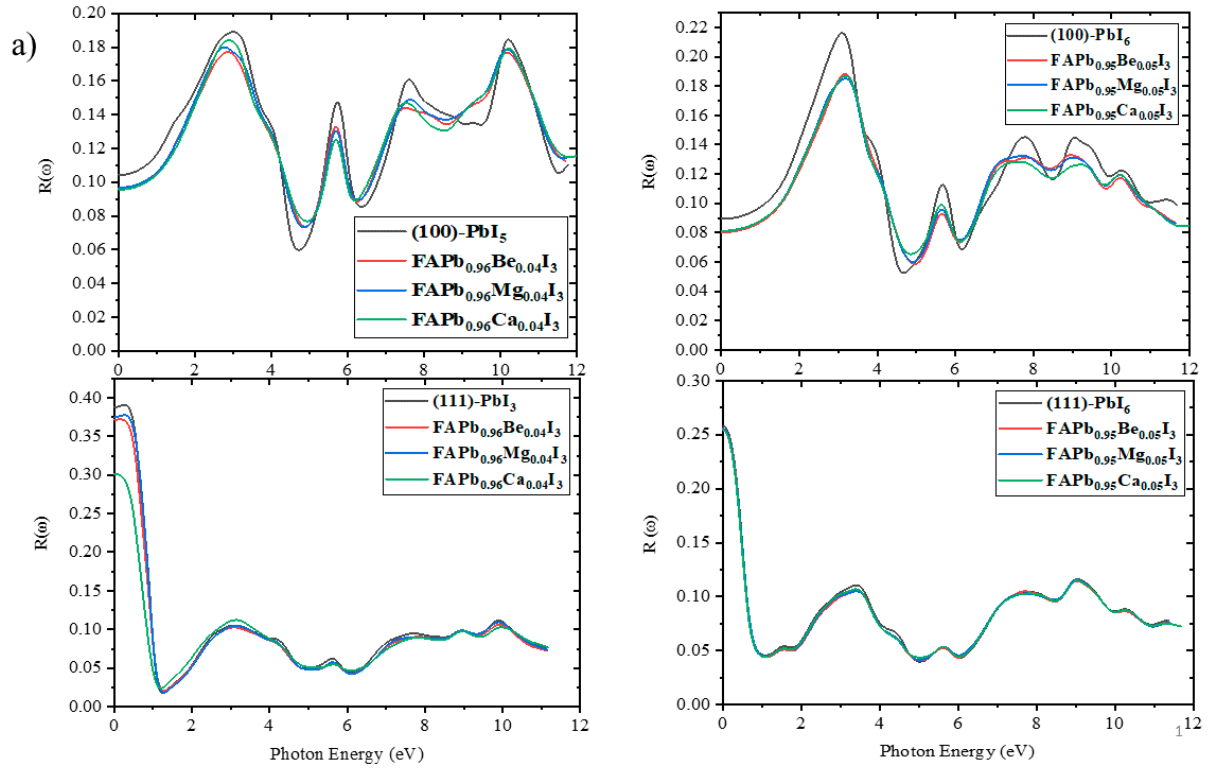


Figure S7. The extinction coefficient for (100) and (111) surfaces with doping of a) 1 atom of Be, Mg, and Ca in all terminations, b) 1-4 atoms of Ca in both PbI₆ terminations and 1-5 atoms of Ca in PbI₅ and PbI₃ terminations, and c) 1-2 atoms of Mg in PbI₃ and PbI₅ terminations.



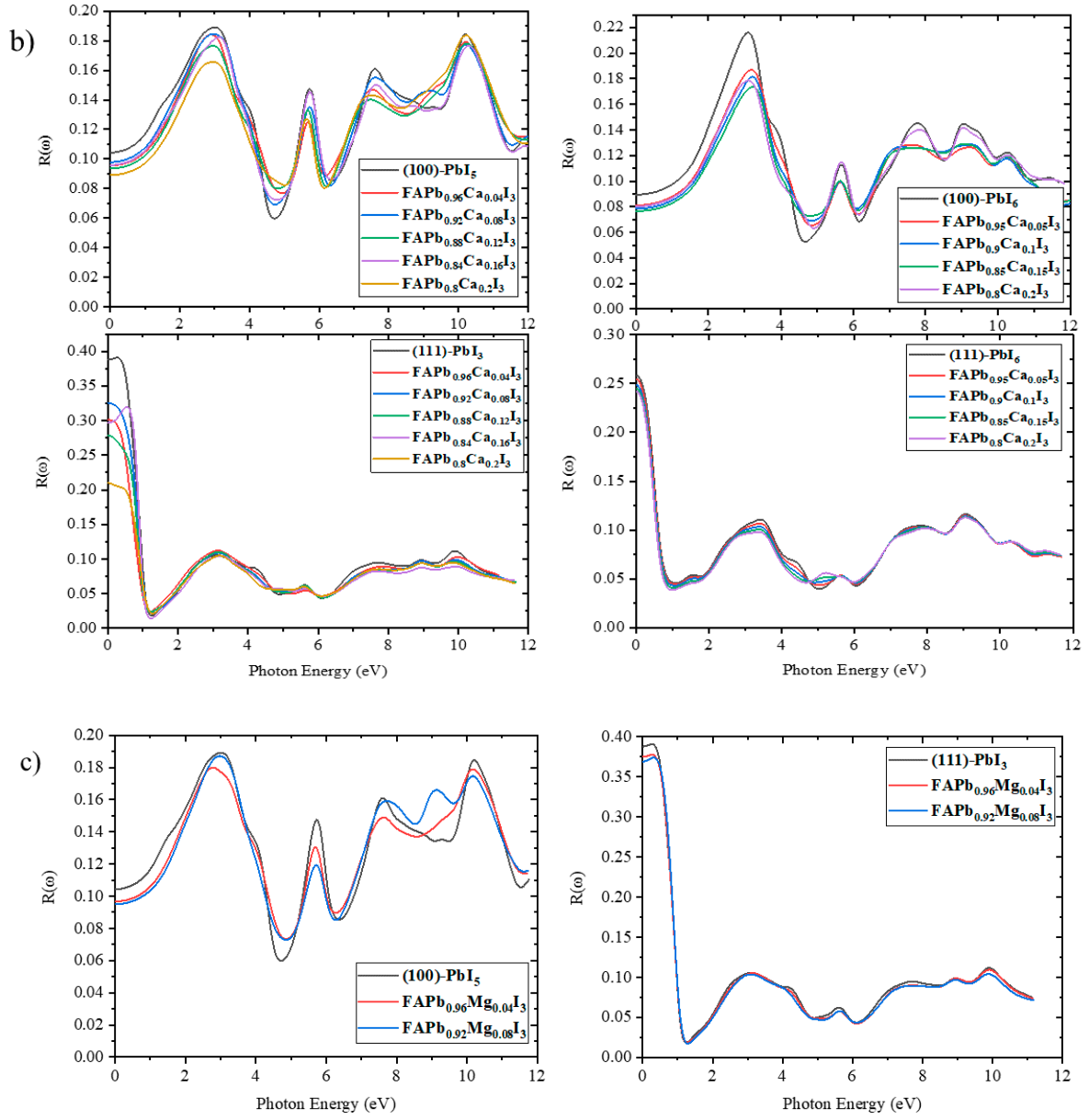
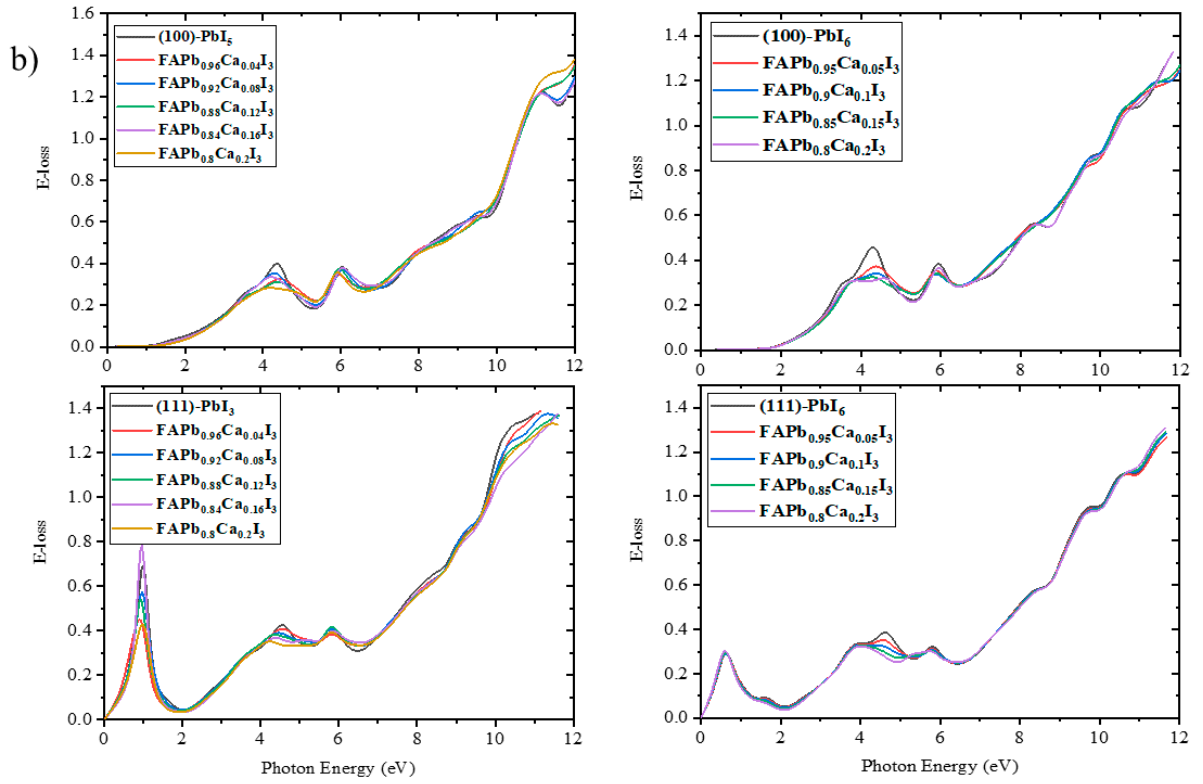
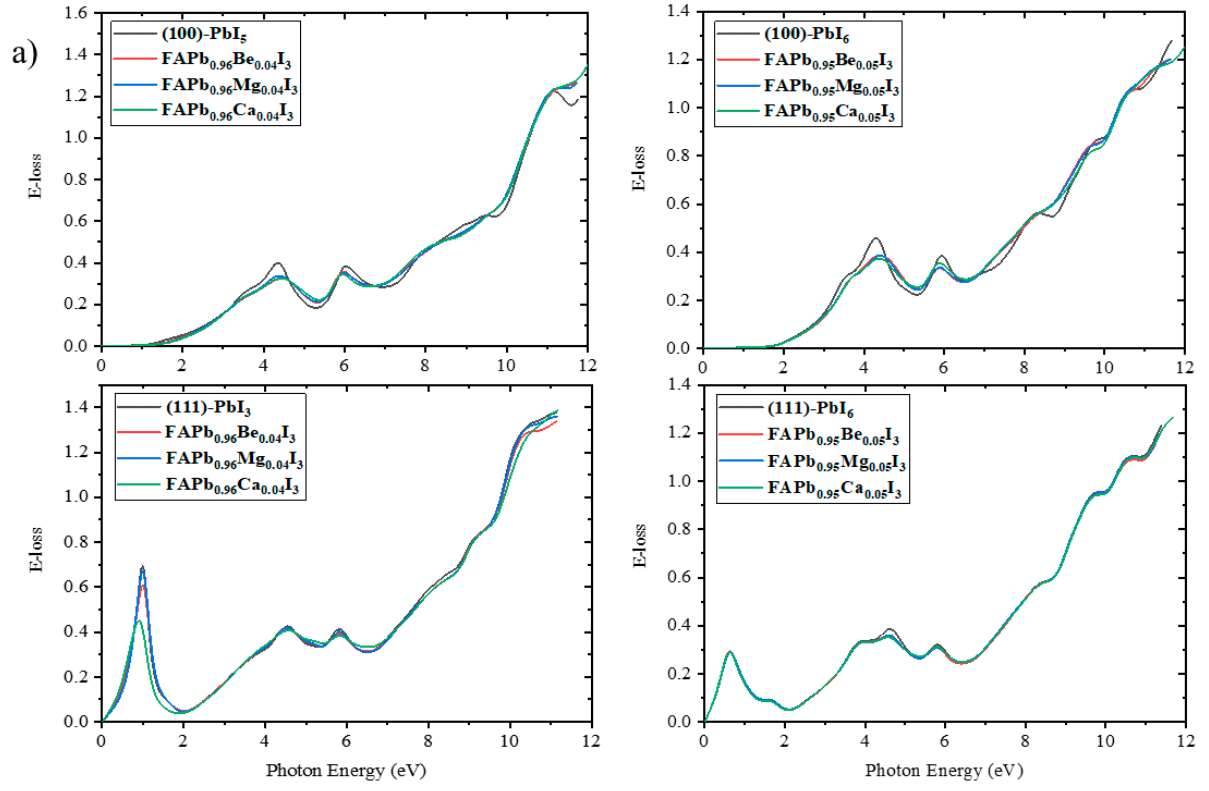


Figure S8. The reflectivity spectra for (100) and (111) surfaces with doping of a) 1 atom of Be, Mg, and Ca in all terminations, b) 1-4 atoms of Ca in both PbI₆ terminations and 1-5 atoms of Ca in PbI₅ and PbI₃ terminations, and c) 1-2 atoms of Mg in PbI₃ and PbI₅ terminations.



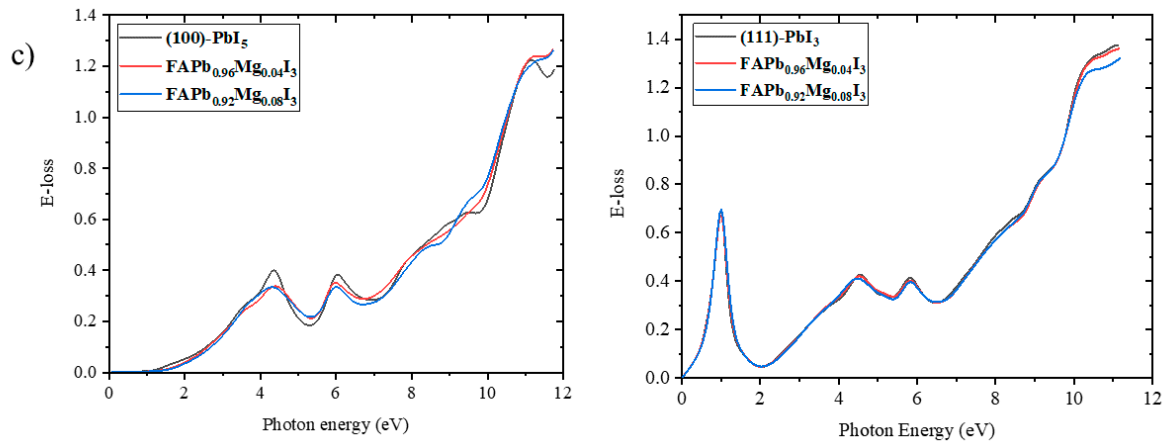


Figure S9. The electron energy loss function versus photon energy for (100) and (111) surfaces with doping of a) 1 atom of Be, Mg, and Ca in all terminations, b) 1-4 atoms of Ca in both PbI_5 terminations and 1-5 atoms of Ca in PbI_5 and PbI_3 terminations, and c) 1-2 atoms of Mg in PbI_3 and PbI_5 terminations.