Supporting Information

A First-Principles Study of Lithium Intercalation and Diffusion in Oxygen-Defective Titanium Dioxide

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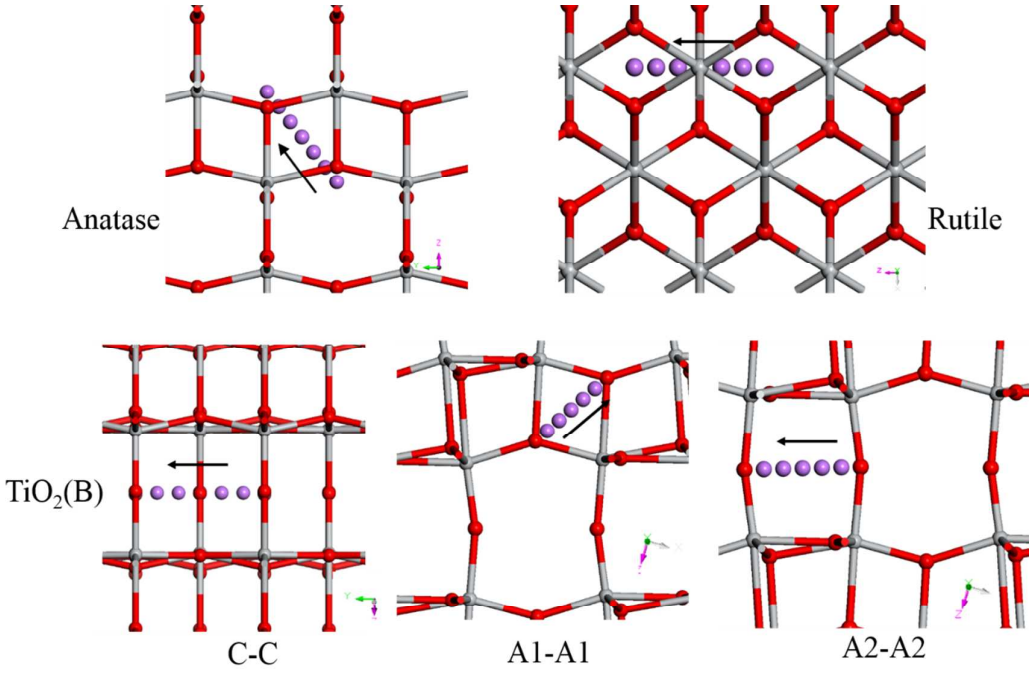

Fig S1. Lithium diffusion pathways for anatase, rutile, and TiO_2(B)

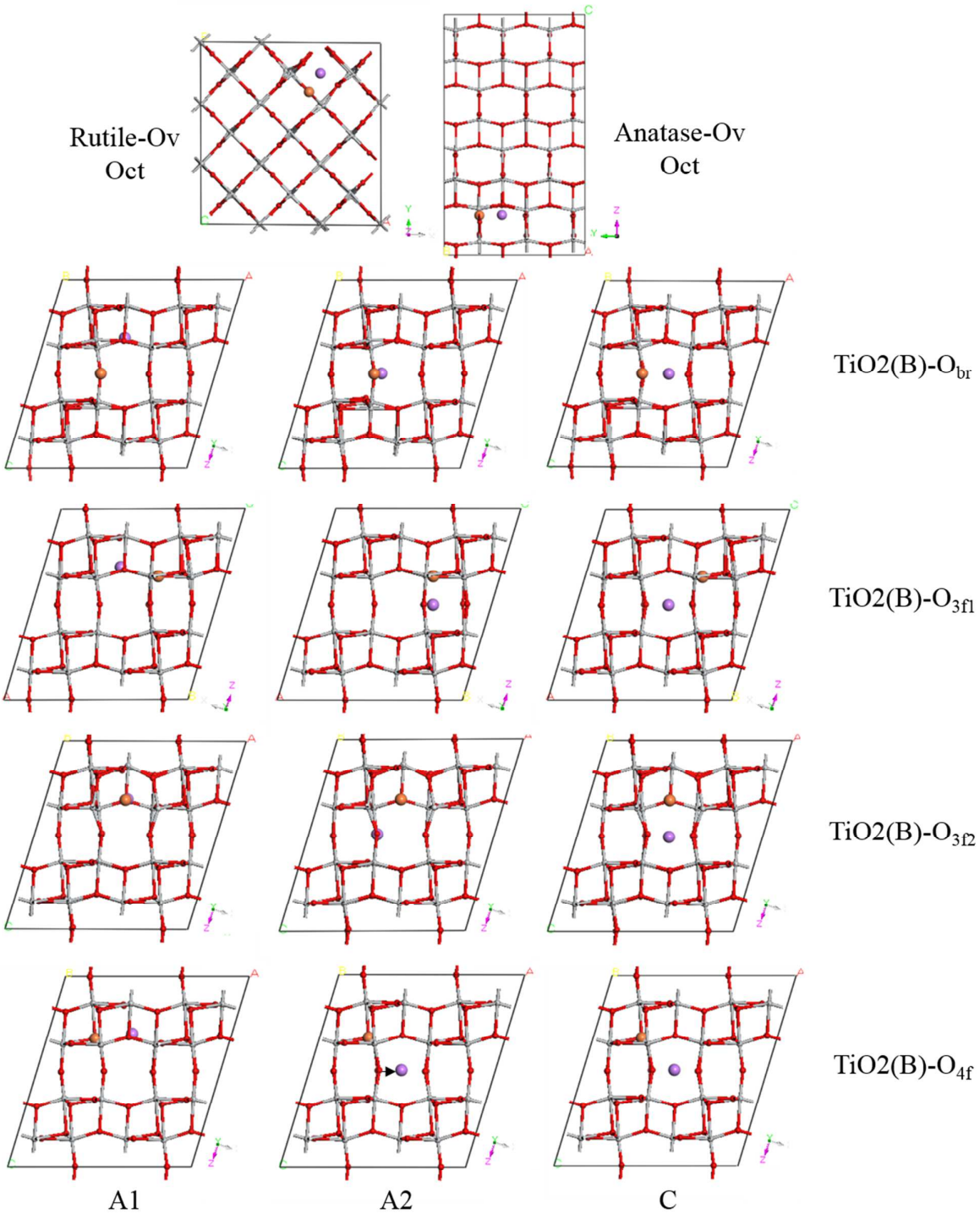

Fig S2. Models of fully geometry optimization for lithium intercalated TiO_2 polymorphs with an oxygen vacancy for the initial position of all considered diffusion paths. Red, gray, and purple spheres represent O, Ti, and Li atoms, respectively. Meanwhile, orange spheres represent possible vacancy sites.

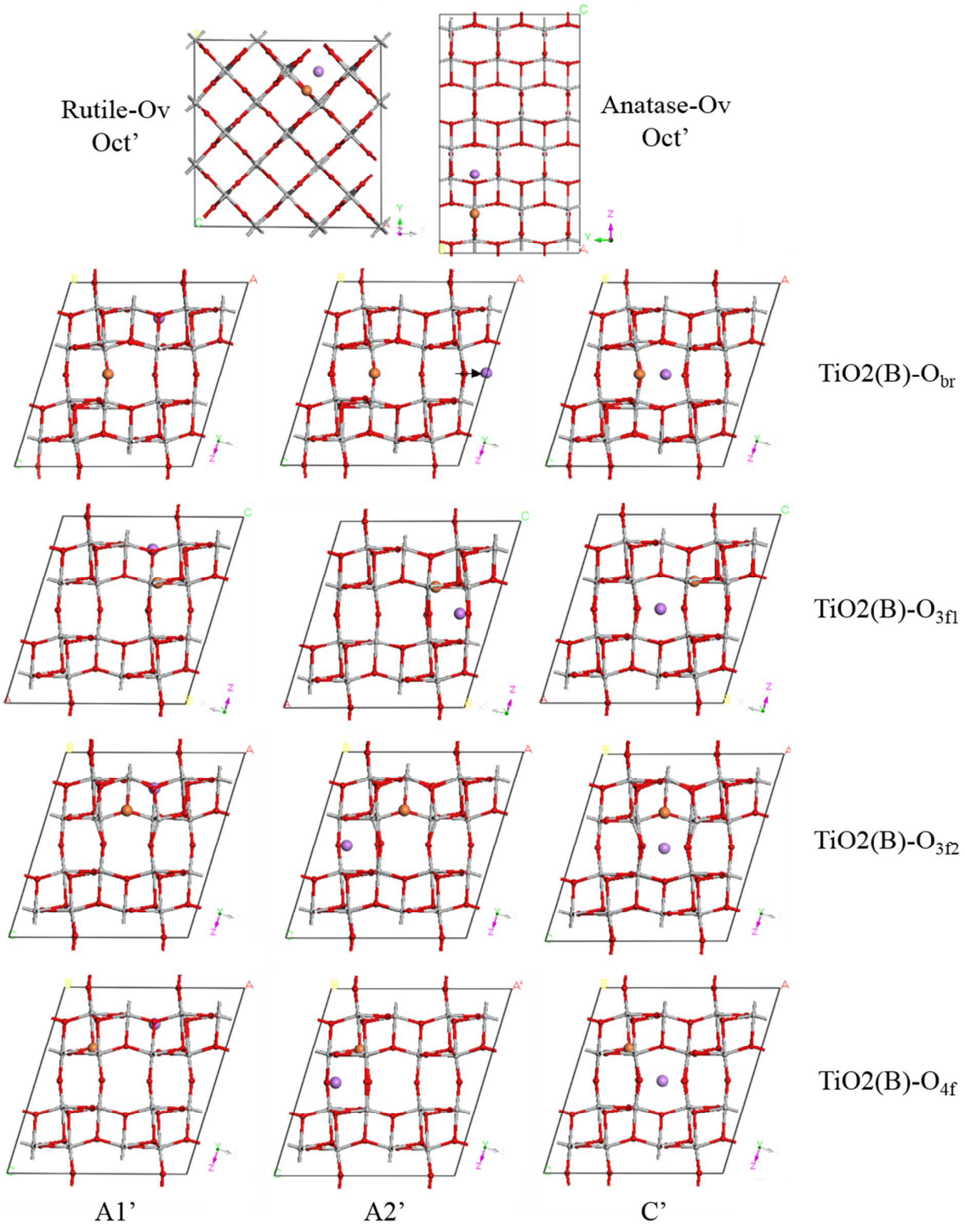

Fig S3. Models of fully geometry optimization for lithium intercalated TiO_2 polymorphs with an oxygen vacancy for the final position of all considered diffusion paths. Red, gray, and purple spheres represent O, Ti, and Li atoms, respectively. Meanwhile, orange spheres represent possible vacancy sites.

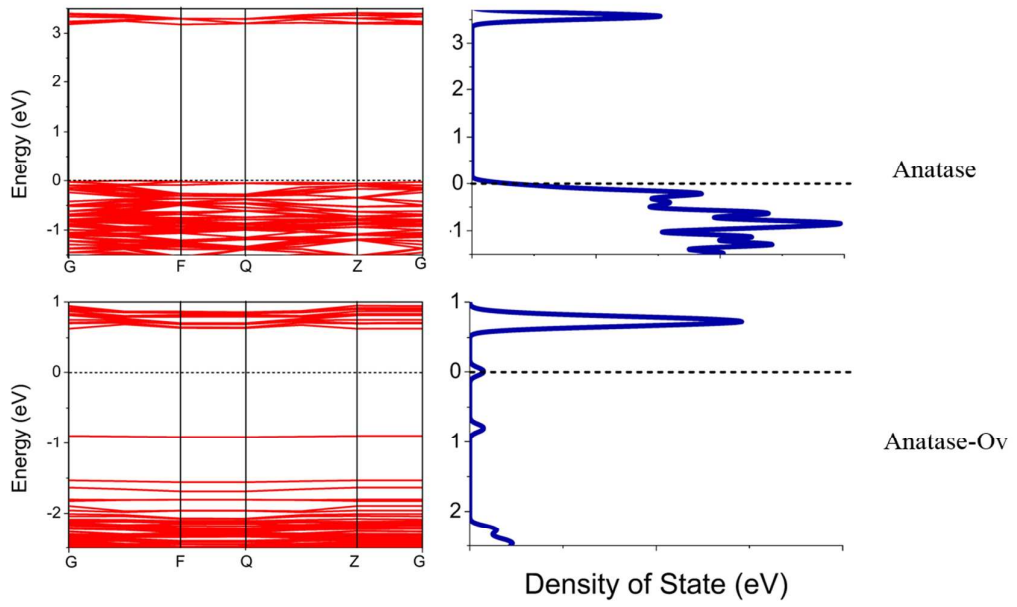

Fig S4. Band structure and DOS analysis for pristine and oxygen-defective anatase.

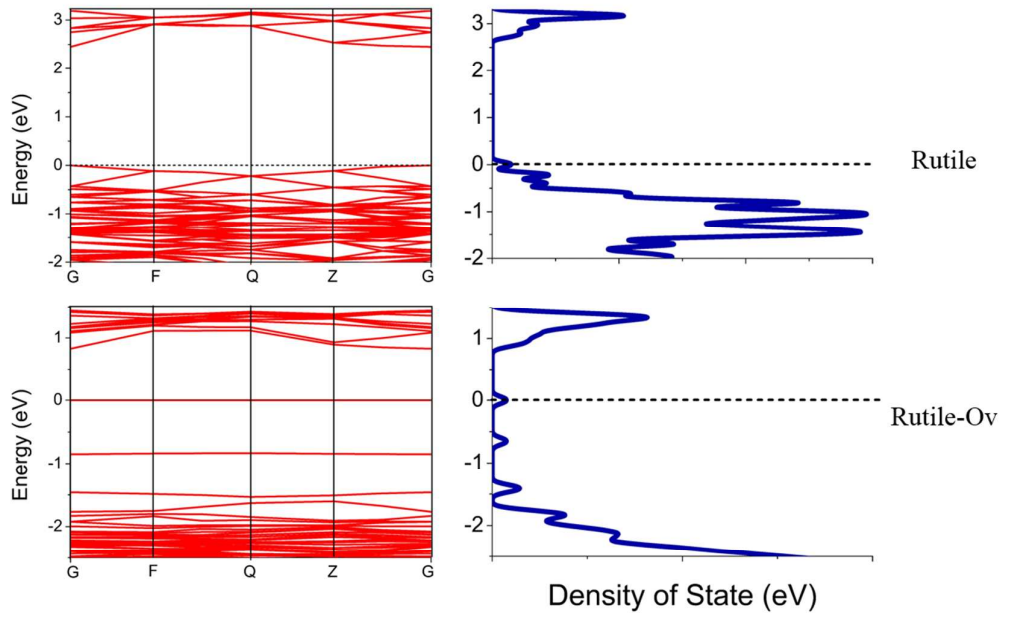

Fig S5. Band structure and DOS analysis for pristine and oxygen-defective rutile.

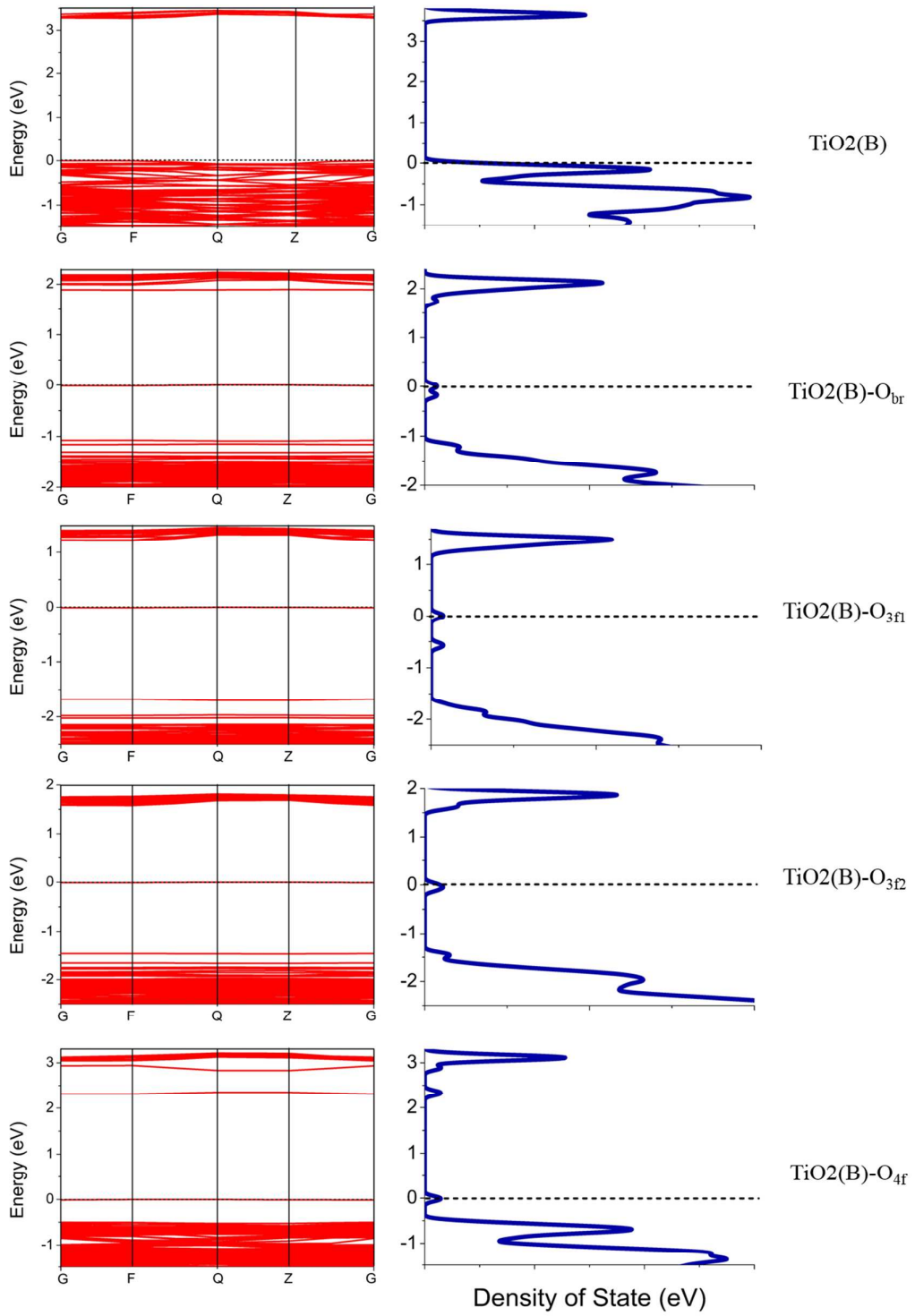

Fig S6. Band structure and DOS analysis for pristine and oxygen-defective TiO_2(B).