Supporting Information

for

Structural and Electronic Properties of Frenkel and Schottky Defects at the MgO{100} Surface: Spin-Polarization, Mid-Band Gap States, and Charge Trapping at Vacancy Sites

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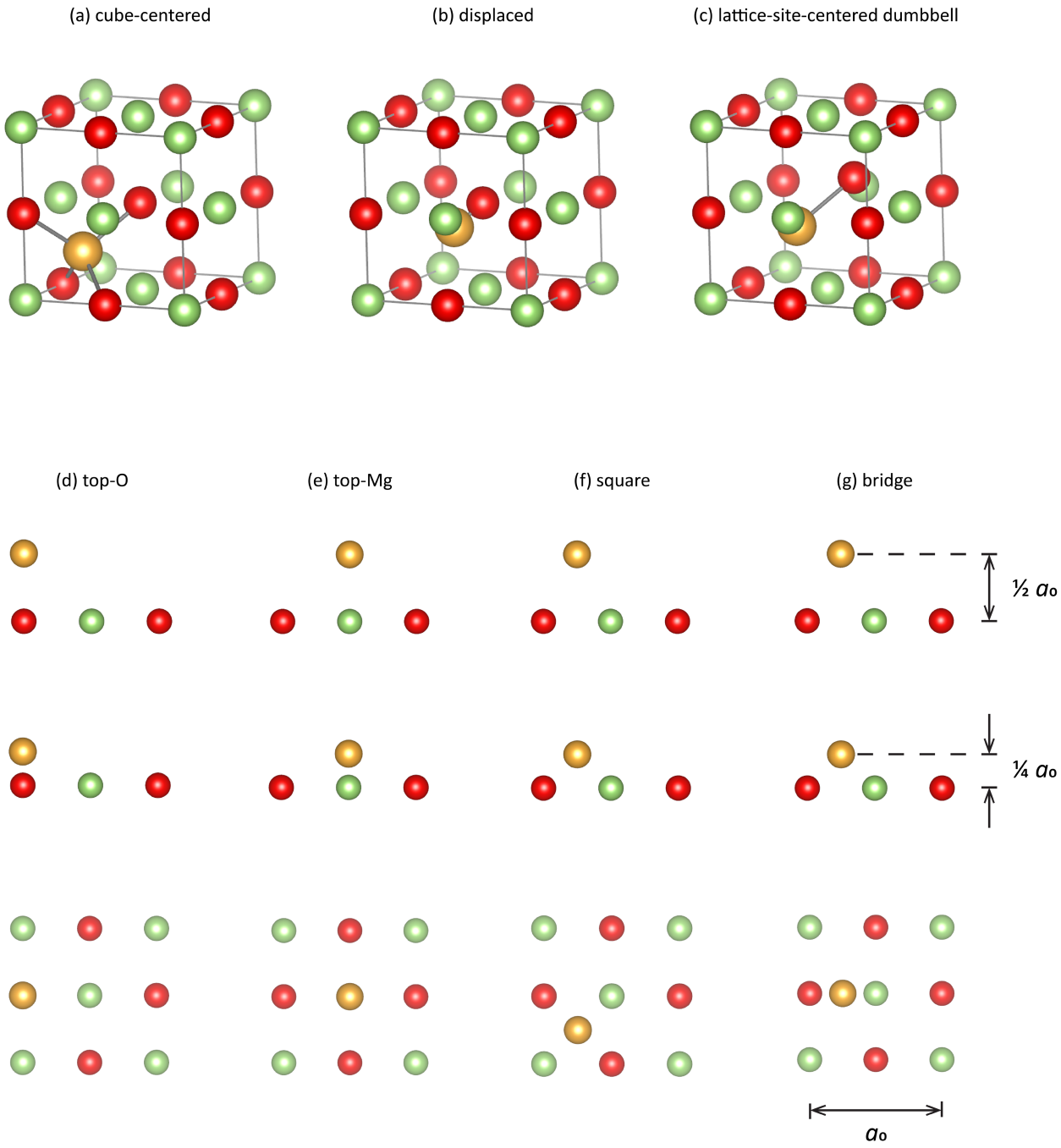

Figure S1. Considered starting positions for Frenkel bulk interstitial atoms (a-c), and Frenkel surface adatoms (d-g). Light green and red spheres denote lattice site Mg and O atoms, respectively. The yellow, slightly larger spheres represent Frenkel interstitials and Frenkel adatoms. Panels (b) and (c) show the displaced and the lattice-site-centered dumbbell starting positions for the O Frenkel interstitial atom. Starting configurations for Mg Frenkel interstitial atoms are constructed analogously.

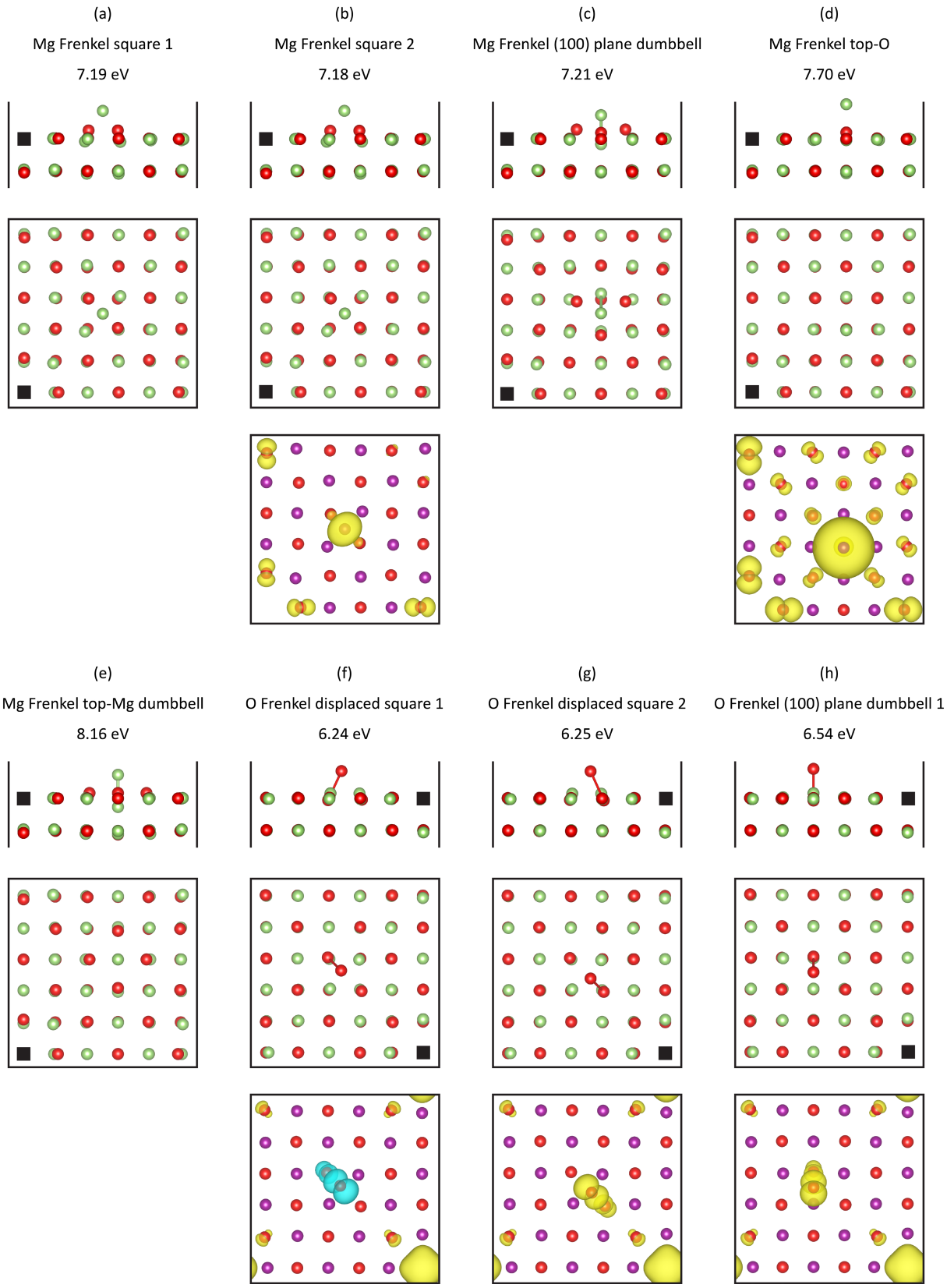

Figure S2. Surface defect output configurations and spin-polarization density plots. See also next page.

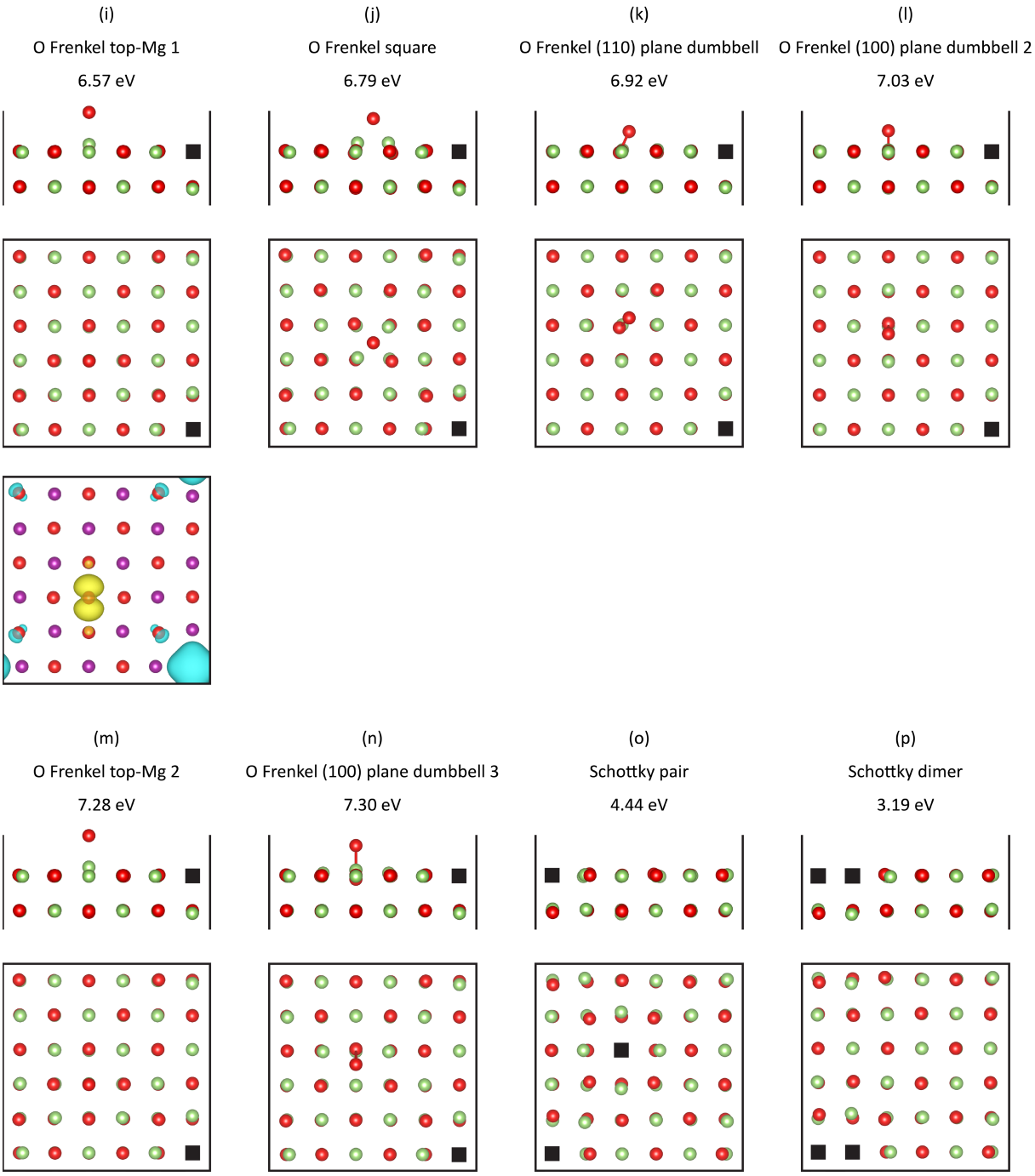

Figure S2 cont. Surface defect output configurations and spin-polarization density plots. The atomic structural models show the two top layers of the Frenkel and Schottky surface defect configurations identified in this study. Light green and red spheres denote Mg and O atoms, respectively. Black squares indicate vacancy sites. The top layer magnetization plots show 0.007 e/Å^3 spin-up minus spin-down electron density isosurfaces for spin-polarized Mg Frenkel configurations, and 0.019 e/Å^3 spin-up minus spin-down electron density isosurfaces for spin-polarized O Frenkel configurations. In these plots, purple and red spheres denote Mg and O atoms, respectively. Net spin-up and net spin-down charge densities are plotted in yellow and blue, respectively. Included are the calculated defect formation energies.

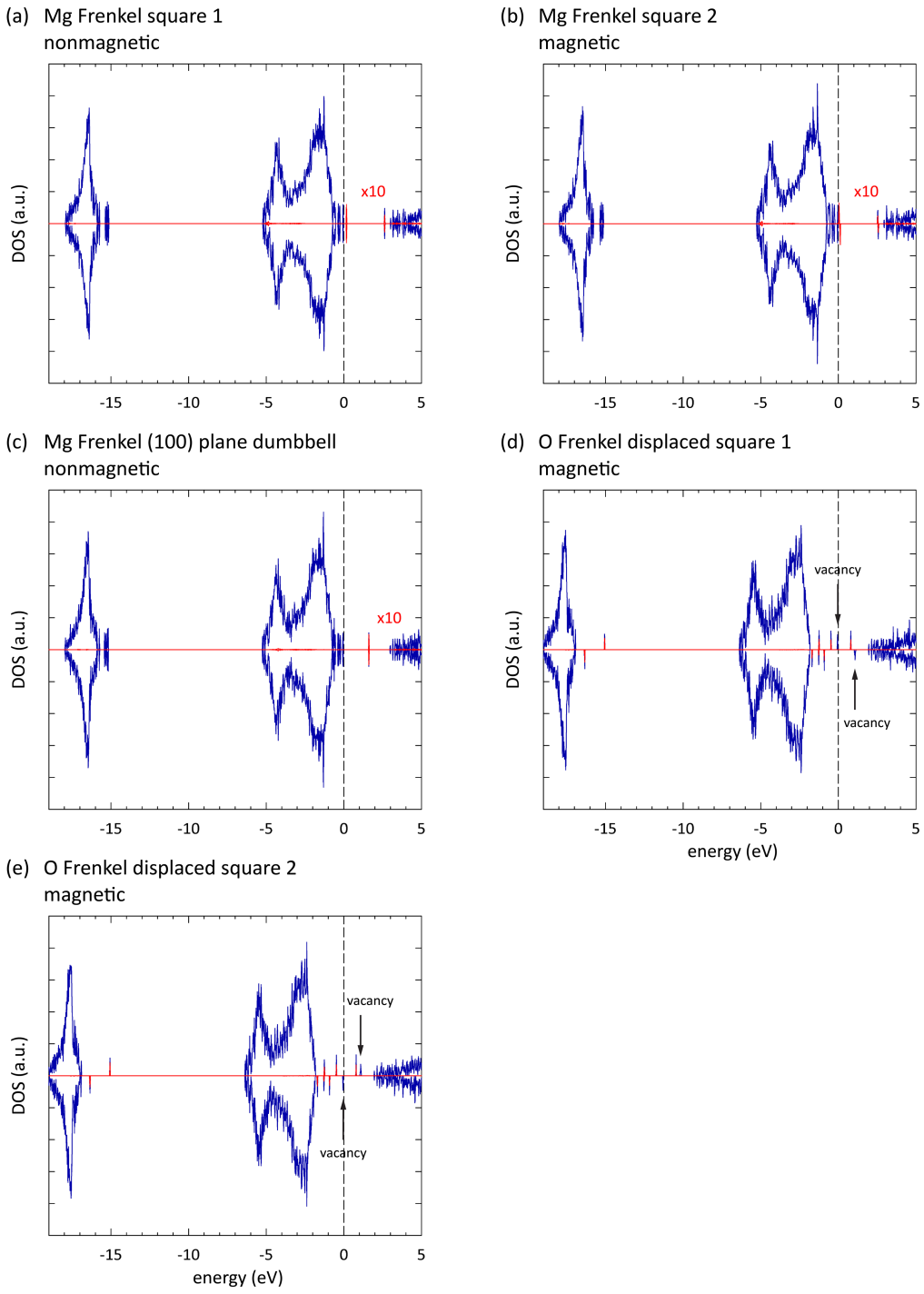

Figure S3. Total and projected density of states (DOS) plots for the lowest-energy Frenkel surface defect configurations identified in this study. Fermi levels are set to zero, and are indicated with a dashed black line. Shown in blue are the total density of majority (spin-up) states, and, in blue and mirrored, the total density of minority (spin-down) states. The projected densities of spin-up and spin-down states for the adatoms are shown in red. Please note that for visualization effects, the projected DOS for the Mg adatoms has been multiplied by 10. Vacancy states are indicated with an arrow.