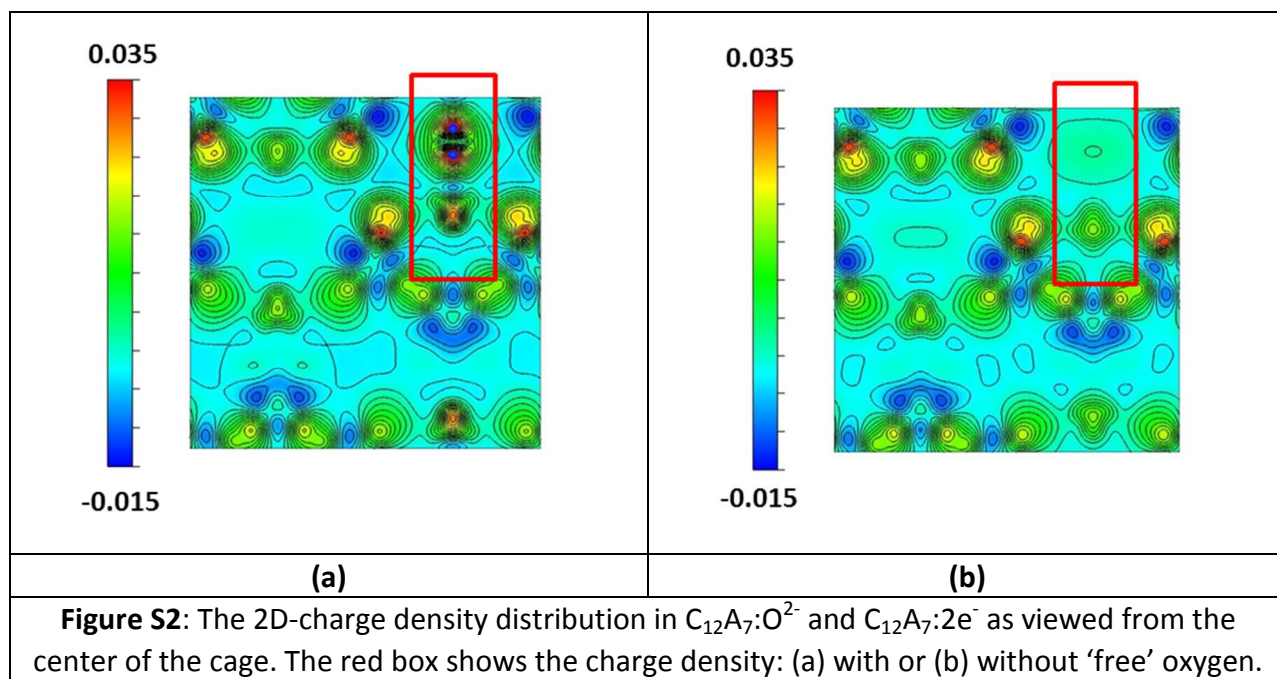
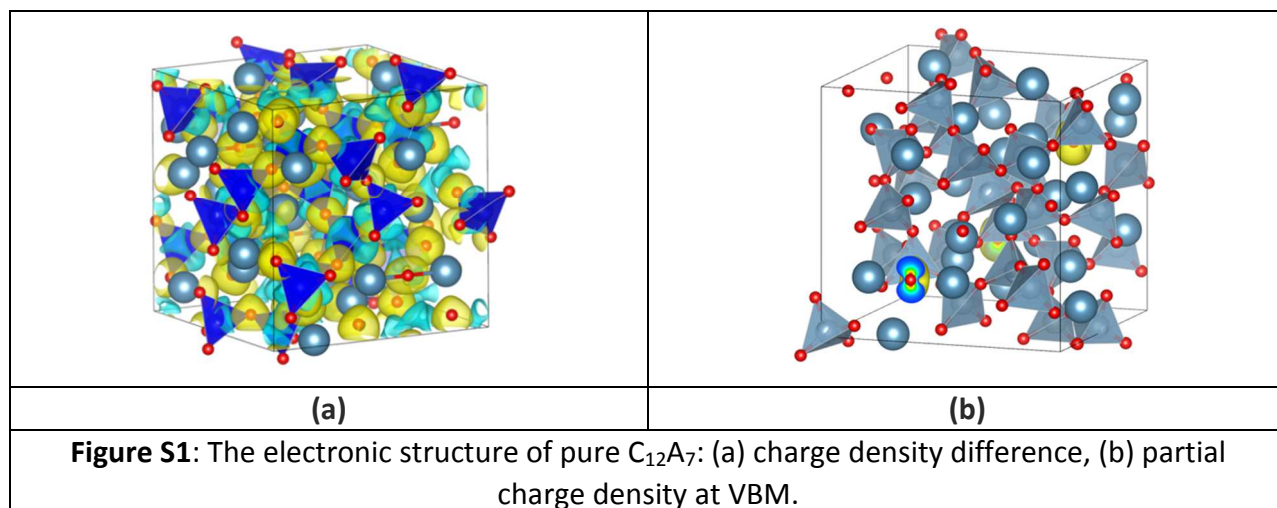
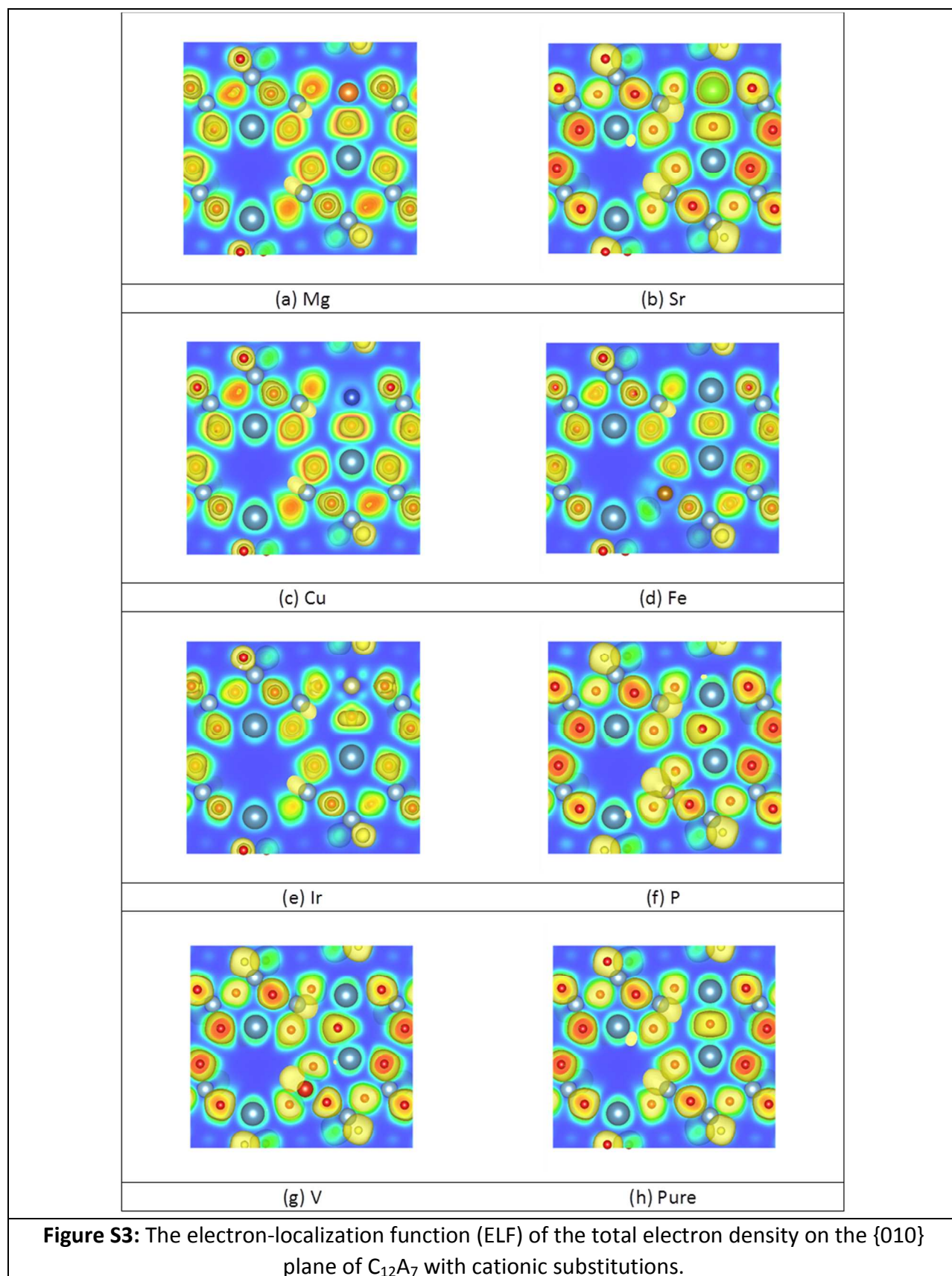


Electronic Supplementary Information (Online Only)





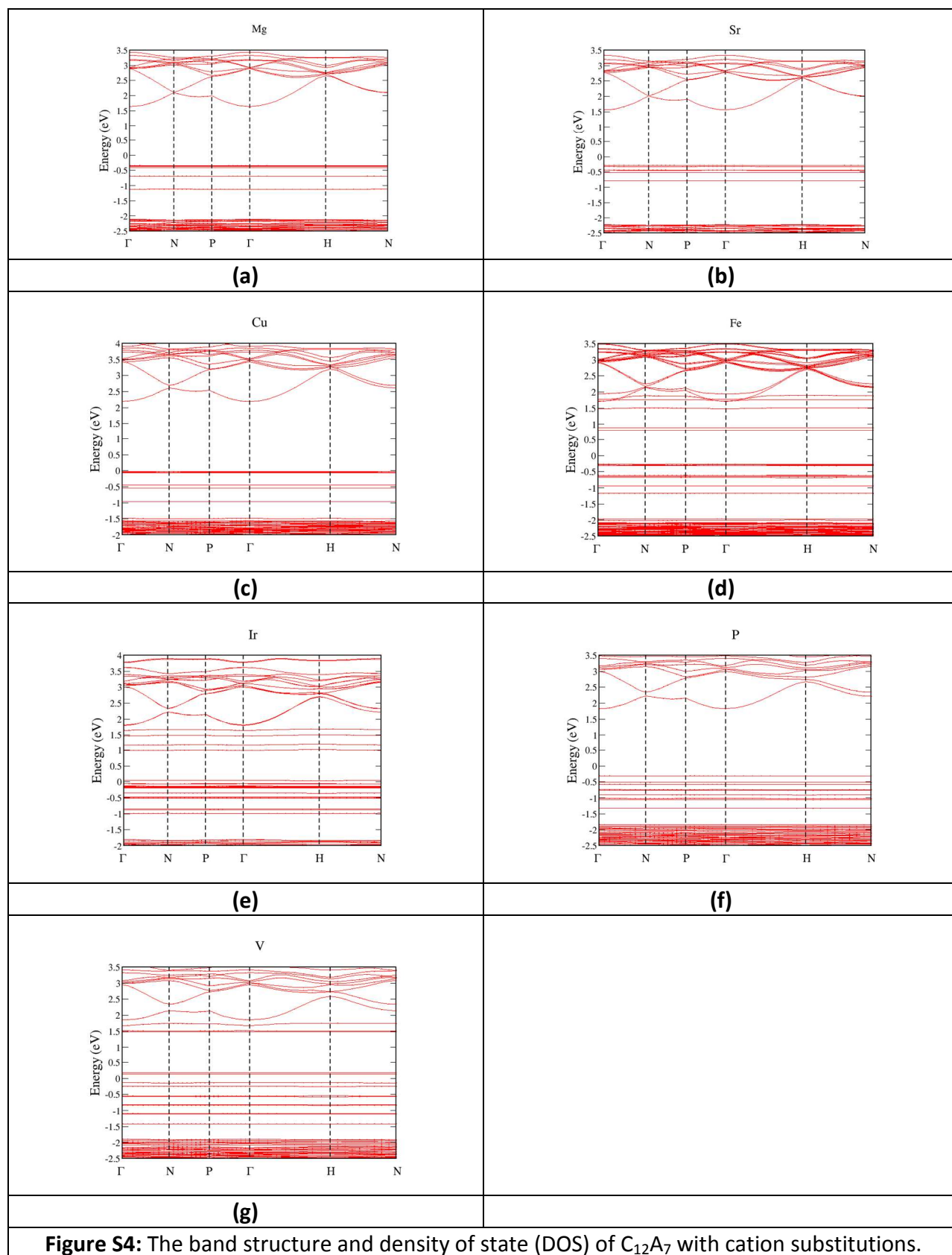


Figure S4: The band structure and density of state (DOS) of $C_{12}A_7$ with cation substitutions.

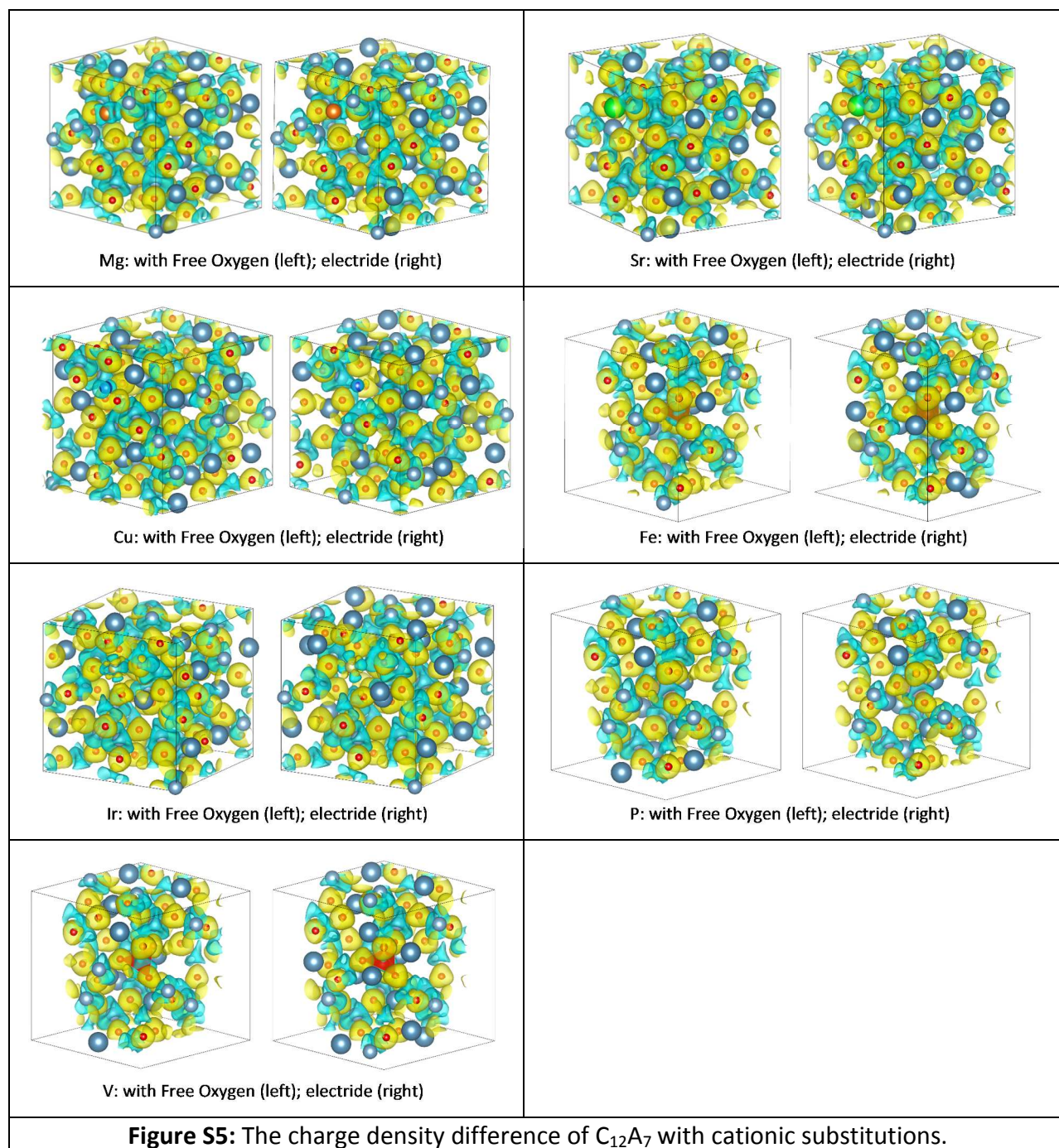


Table S1: The Bader charges and ELF values for Cu and Ir doped C₁₂A₇ variants						
	Ca	Al	O	Free O	Impurity	ELF max.
Pure	1.57	2.44	-1.56	-1.36, -1.46	-	0.8612
electride	1.56	2.43	-1.58	-	-	0.9110
Mg	1.51-1.57	2.43	-1.57-1.62	-1.37, -1.47	1.71	0.7980
electride	1.47-1.56	2.43	-1.59-1.64	-	1.11	0.9815
Cu	1.52-1.57	2.44	-1.56-1.62	-1.06, -1.28	0.83	0.8625
electride	1.56	2.44	-1.57-1.63	-	-0.56	0.8638
Sr	1.50-1.57	2.44	-1.57-1.63	-1.36, -1.38	1.55	0.8622
electride	1.43-1.56	2.44	-1.59-1.63	-	1.39	0.9415
Fe	1.51-1.57	2.44	-1.38-1.62	-1.37,-1.36	1.51	0.7121
electride	1.53-1.55	2.43	-1.57-1.64	-	0.87	0.7140
Ir	1.53-1.56	2.43	-1.56-1.62	-1.34, -0.88, -1.32	1.42	0.7585
electride	1.54-1.56	2.43	-1.50-1.63	-	-0.34	0.7166
V	1.53-1.57	2.44	-1.21-1.63	-1.41, -1.39, -1.38	2.09	0.8661
electride	1.50-1.56	2.43	-1.53-1.65	-	1.17	0.8776
P	1.53-1.57	2.44	-1.56-1.62	-1.41, -1.39, 1.41	3.67	0.8733
electride	1.51-1.56	2.43	-1.64-1.66	-	3.64	0.8695

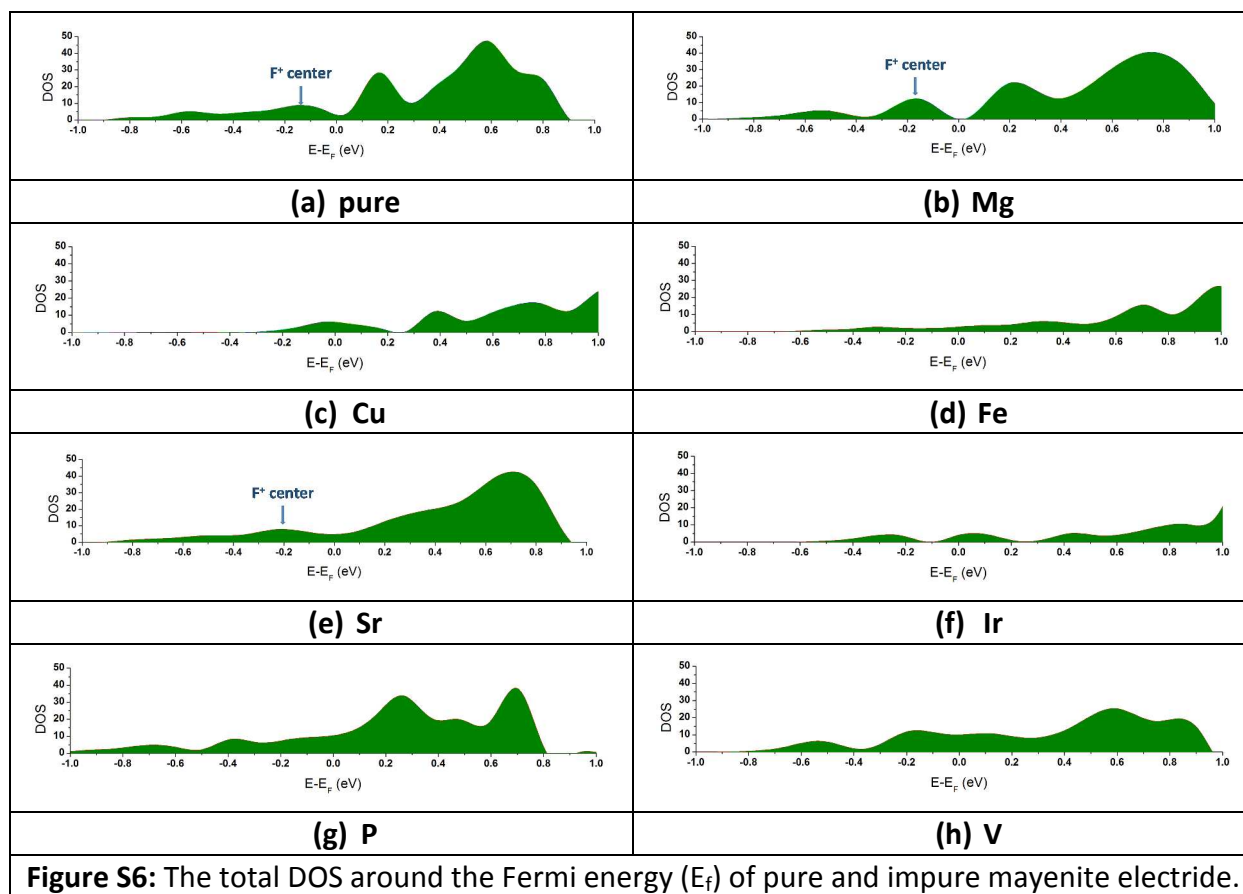
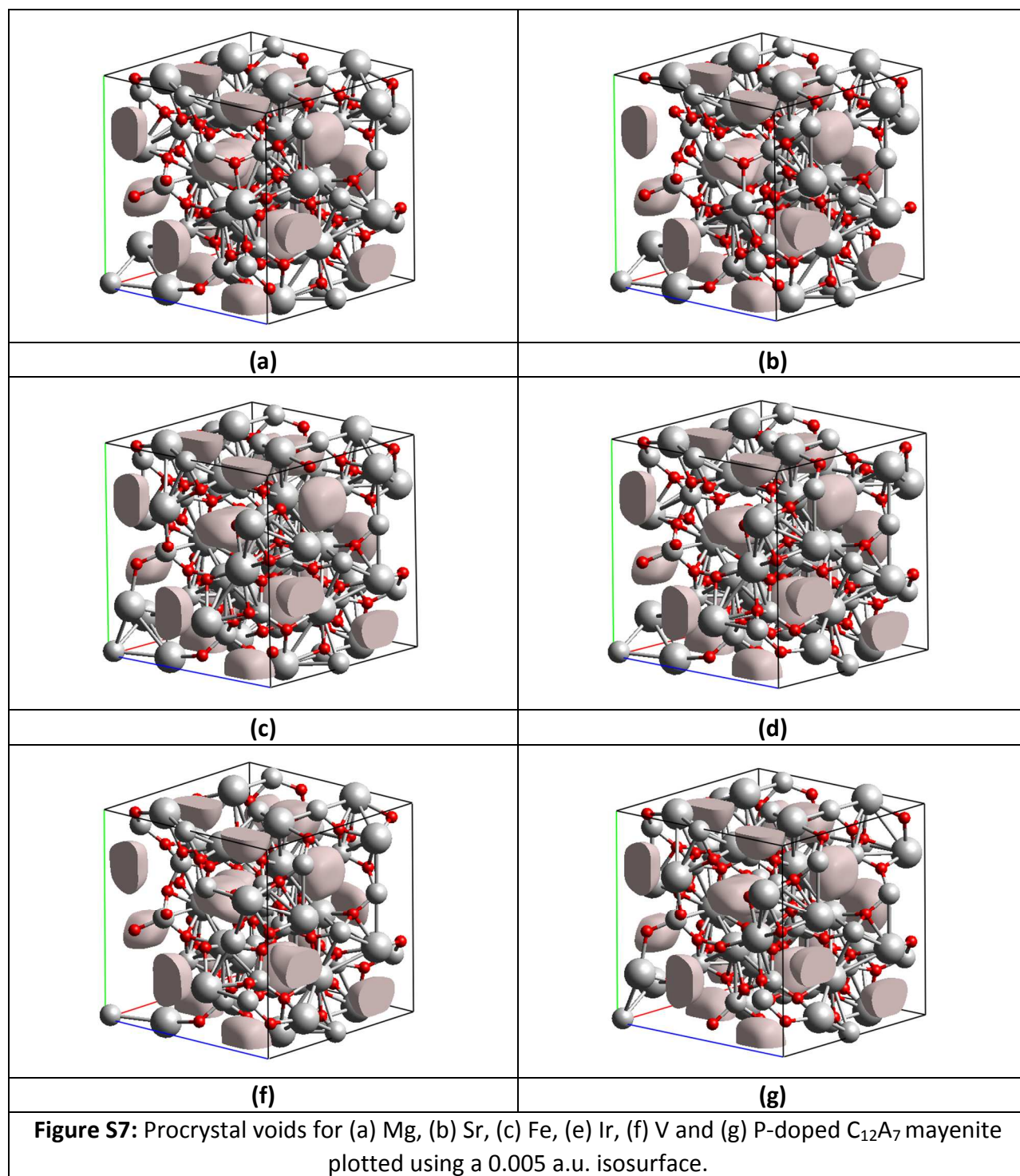


Figure S6: The total DOS around the Fermi energy (E_f) of pure and impure mayenite electride.



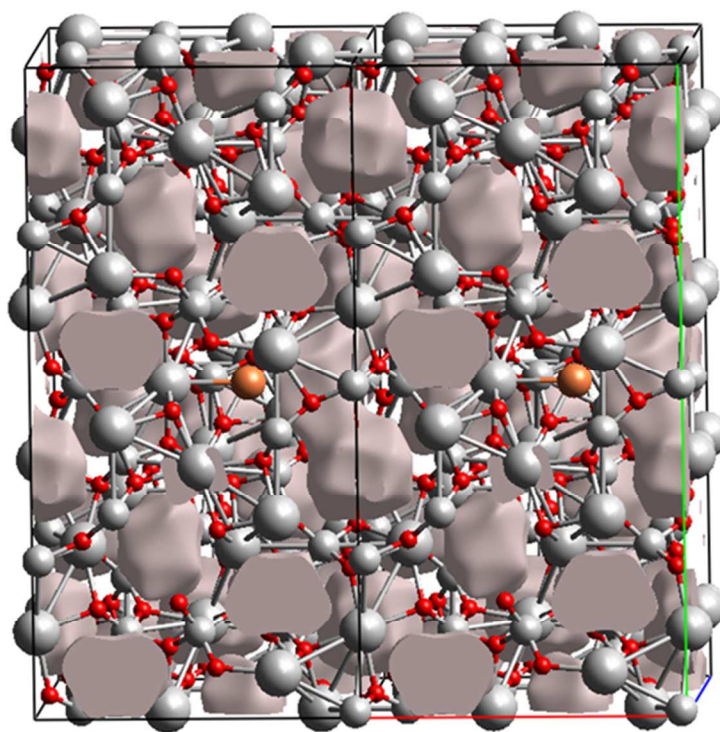


Figure S8: Procrystal voids for Cu-doped C₁₂A₇ mayenite (1 X 2 X 1 supercell) plot using a 0.01 a.u. isosurface. Repeating one unit cell along the x-axis clarifies the persistence of the channel.