

Ab initio insight into the interaction of metal-decorated fluorinated carbon fullerenes with anti-COVID drugs

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SUPPLEMENTARY MATERIALS

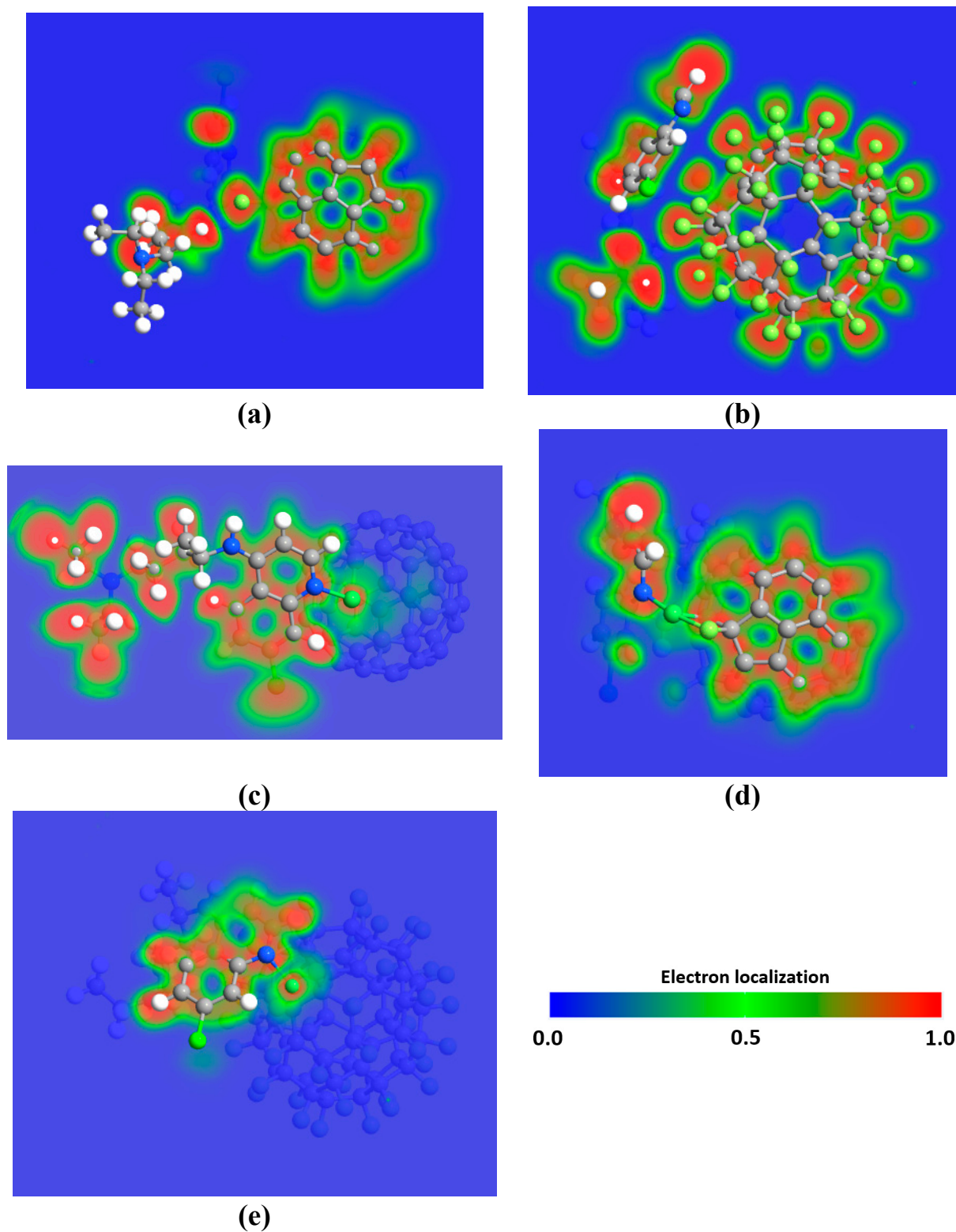
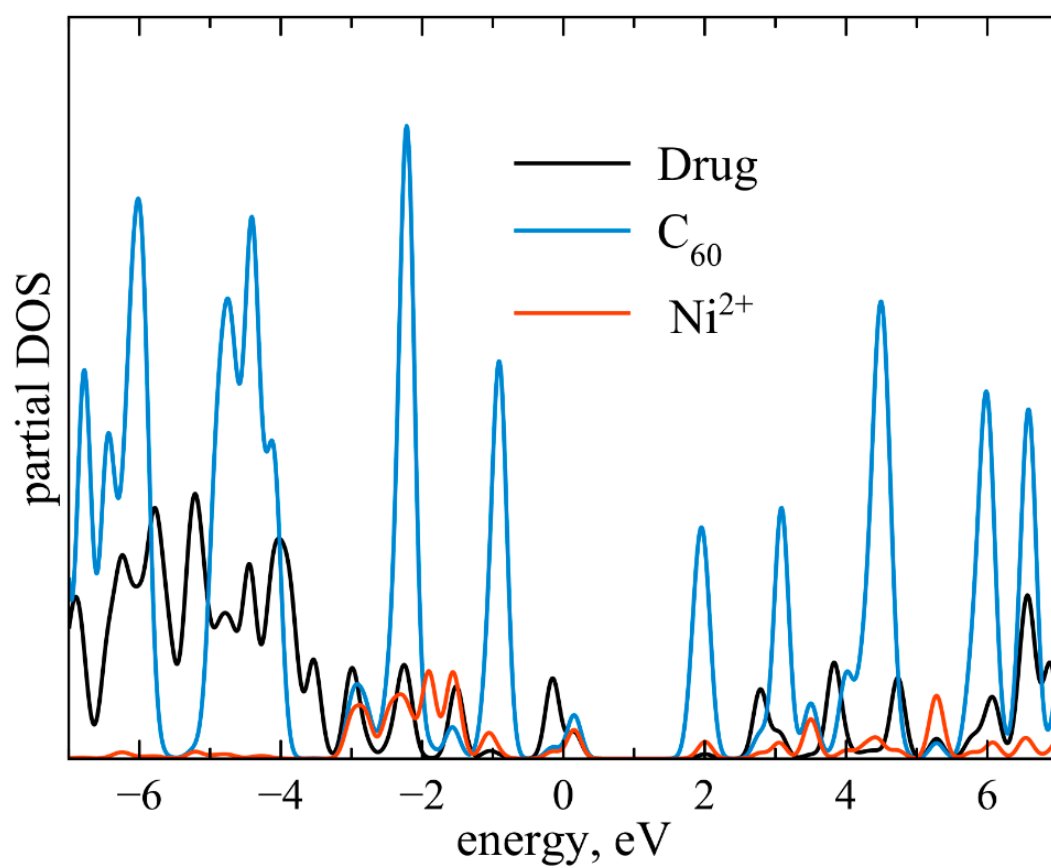
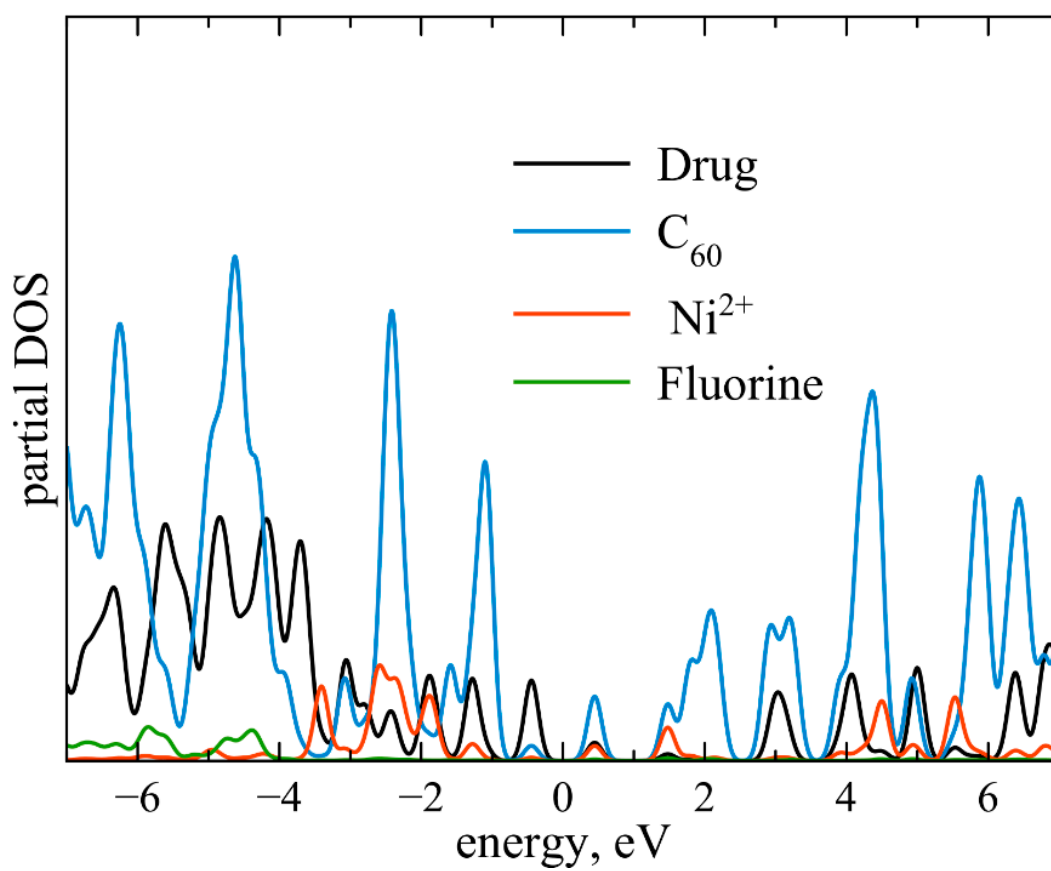


Figure S1. Electron localization function calculated for chloroquine drug loaded on (a) $C_{60}F_2$, (b) $C_{60}F_{48}$, (c) $C_{60}Ni^{2+}$, (d) $C_{60}F_2Ni^{2+}$, and (e) $C_{60}F_{48}Ni^{2+}$. Figure is plotted with Quantum ATK software [54].



(a)



(b)

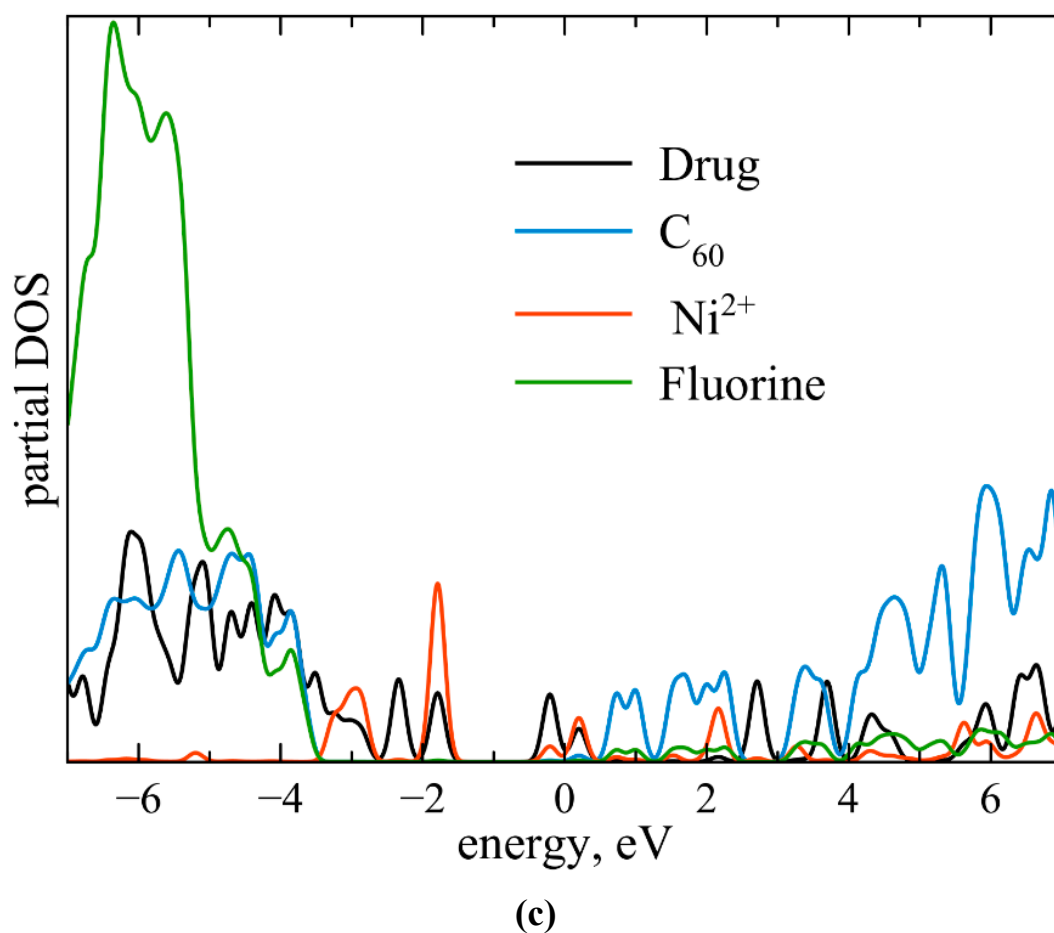


Figure S2. Partial densities of state calculated for chloroquine drug loaded on (a) $C_{60}Ni^{2+}$, (b) $C_{60}F_2Ni^{2+}$, and (c) $C_{60}F_{48}Ni^{2+}$. Zero energies correspond to the arithmetic mean of the frontier HOMO and LUMO orbitals. The calculated energies of molecular orbitals are broadened by Gaussian curves with $\sigma = 0.1$ eV.