Supplementary Materials

for

Electronic and reactivity characteristics of CL-20 covalent chains and networks: A density functional theory study

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Table S1. Binding energy (E_b), HOMO energy (ε_H), LUMO energy (ε_L), ionization potential (IP), electron affinity (EA), HOMO-LUMO gap (Δ_{HL}), chemical potential (μ), electronegativity (χ), hardness (η), softness (S), electrophilicity (ω), maximum electronic charge accepted (ΔN_{max}), and dipole moment (μ_D) of CL-20 covalent low-dimensional nanostructures obtained at DFT/PBE0/6-311(d,p) level of theory

Chain / Network	E_b, eV/atom	ε_H, eV	ε_L, eV	IP, eV	EA, eV	Δ_{HL}, eV	μ, eV	χ, eV	η, eV	S, eV^{-1}	ω, eV	ΔN_{max}, a.u.	μ_D, D/fragment
1×1	4.158	-9.177	-2.844	9.177	2.844	6.333	-6.010	6.010	3.167	0.158	5.704	1.898	1.099
2×1	4.291	-7.789	-2.522	7.789	2.522	5.266	-5.155	5.155	2.633	0.190	5.046	1.958	0.049
3×1	4.346	-7.134	-2.430	7.134	2.430	4.704	-4.782	4.782	2.352	0.213	4.861	2.033	0.596
4×1	4.370	-6.904	-2.398	6.904	2.398	4.506	-4.651	4.651	2.253	0.222	4.800	2.064	0.298
5×1	4.384	-6.819	-2.367	6.819	2.367	4.451	-4.593	4.593	2.226	0.225	4.739	2.064	0.548
6×1	4.395	-6.733	-2.357	6.733	2.357	4.376	-4.545	4.545	2.188	0.229	4.721	2.077	0.018
3×2	4.437	-6.915	-2.359	6.915	2.359	4.555	-4.637	4.637	2.278	0.220	4.720	2.036	0.014
4×2	4.434	-6.521	-2.374	6.521	2.374	4.148	-4.447	4.447	2.074	0.241	4.769	2.145	0.006
5×2	4.480	-6.256	-2.099	6.256	2.099	4.157	-4.177	4.177	2.079	0.241	4.197	2.010	0.409
6×2	4.435	-6.355	-2.338	6.355	2.338	4.017	-4.346	4.346	2.009	0.249	4.703	2.164	0.007
4×3L	4.467	-6.245	-2.298	6.245	2.298	3.946	-4.271	4.271	1.973	0.253	4.624	2.165	0.005
4×3Z	4.438	-6.202	-2.289	6.202	2.289	3.913	-4.245	4.245	1.957	0.256	4.606	2.170	0.055

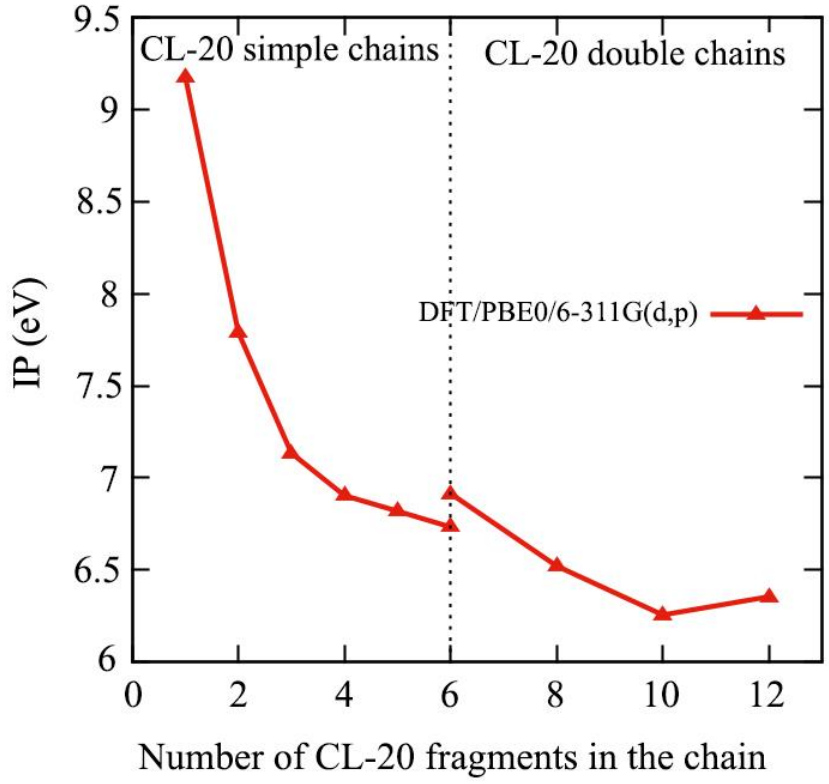


Fig. S1. Ionization potential versus the number of CL-20 fragments in the system obtained at the DFT/PBE0/6-311(d,p) level of theory

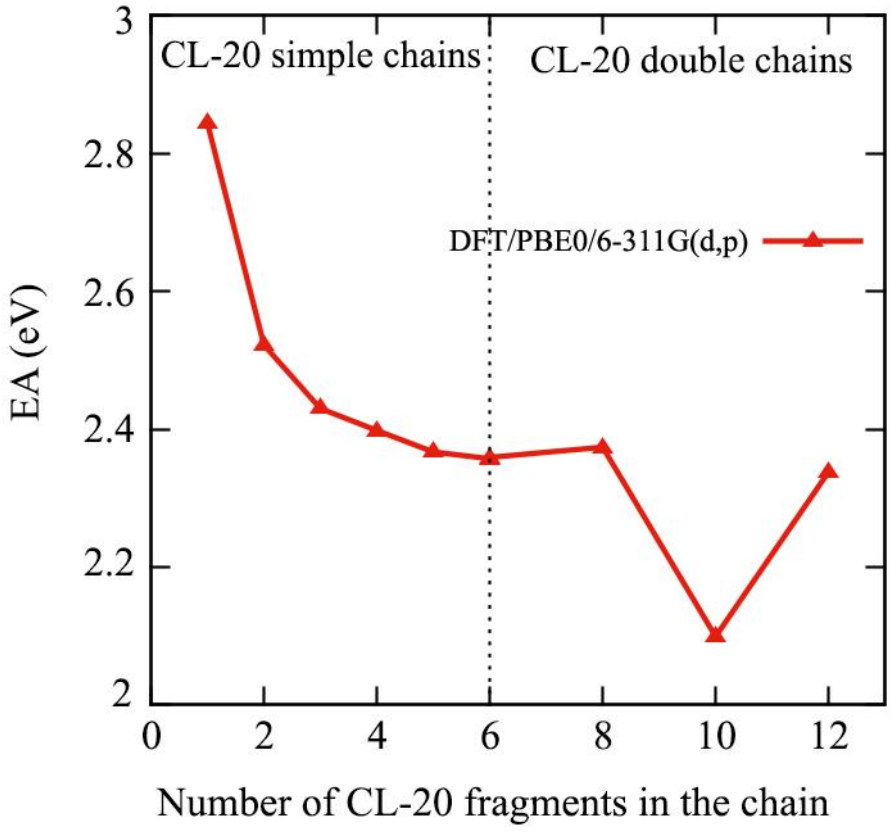


Fig. S2. Electron affinity versus the number of CL-20 fragments in the system obtained at the DFT/PBE0/6-311(d,p) level of theory

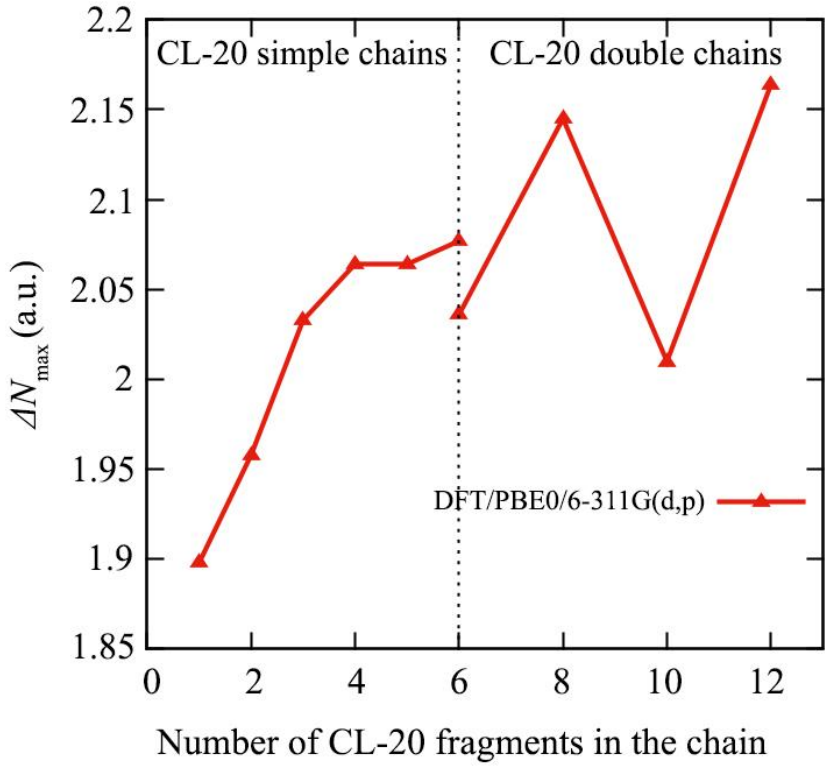


Fig. S3. Maximum electronic charge accepted versus the number of CL-20 fragments in the system obtained at the DFT/PBE0/6-311(d,p) level of theory

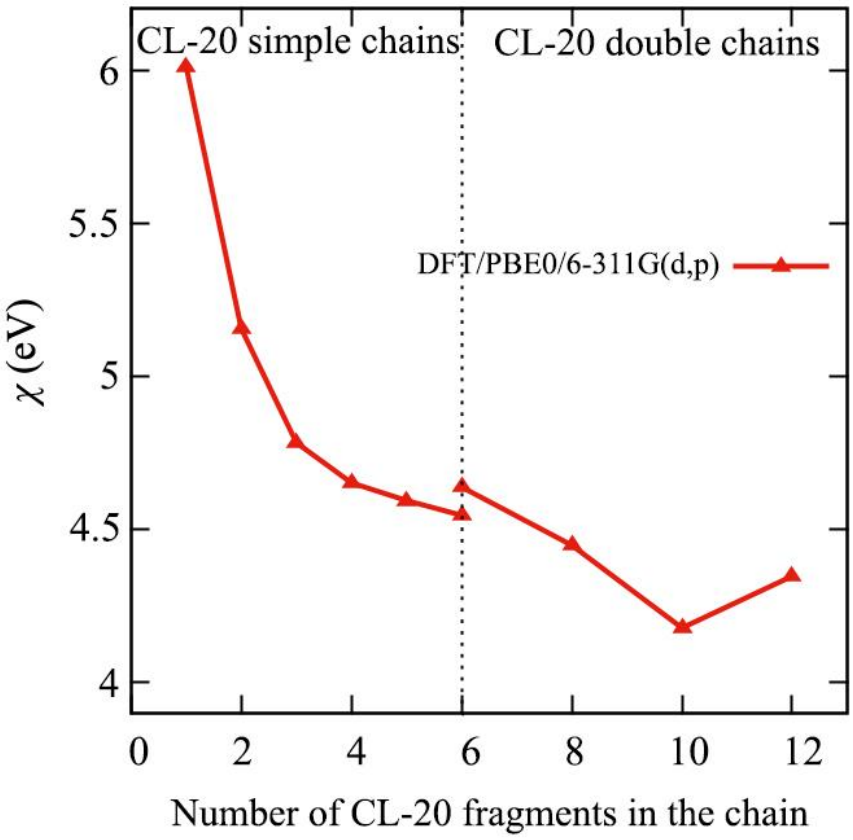
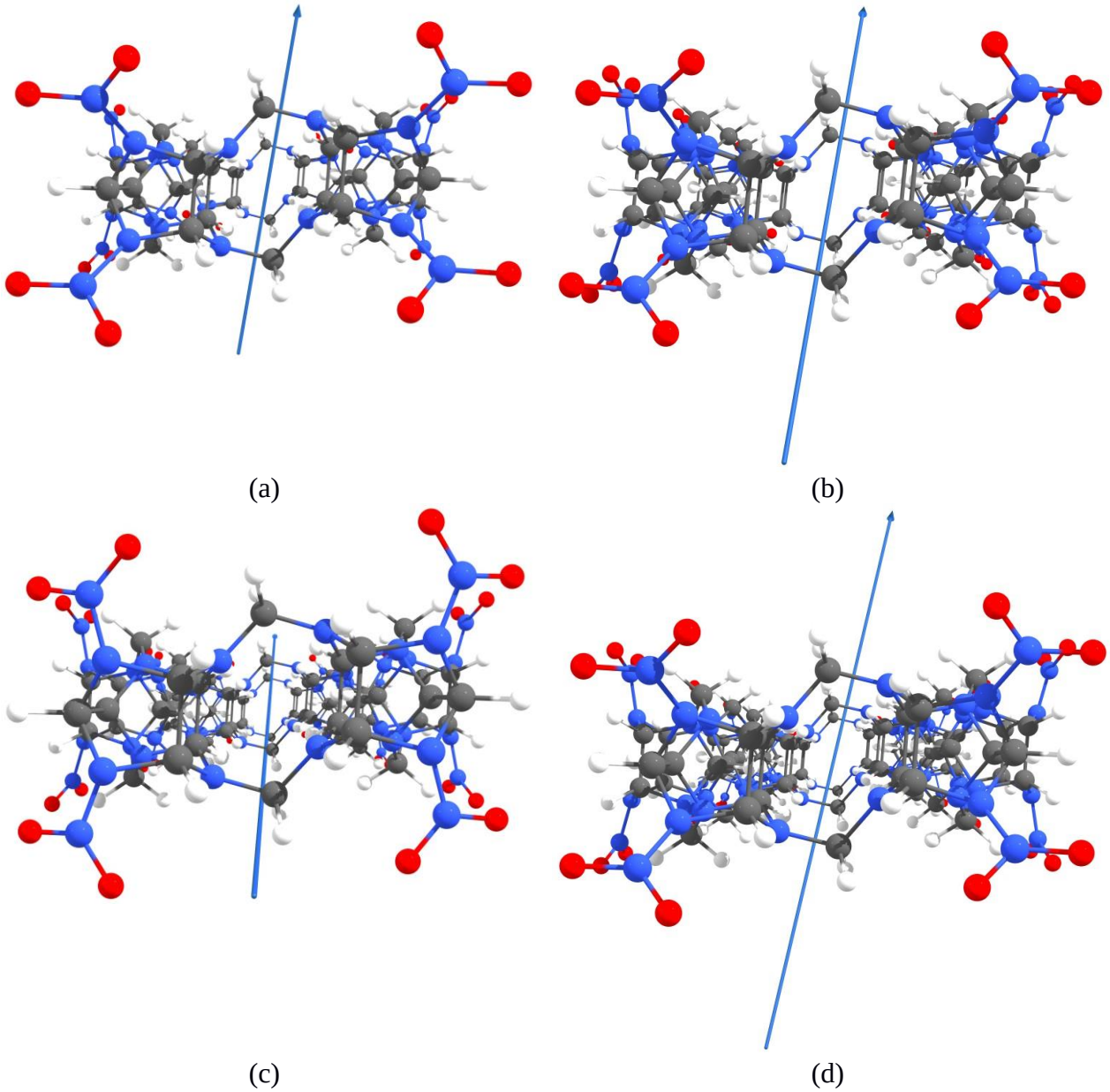


Fig. S4. Electronegativity versus the number of CL-20 fragments in the system obtained at the DFT/PBE0/6-311(d,p) level of theory



(a) (b)

(c) (d)

Fig. S5. Perspective view of 3×2 (a), 4×2 (b), 5×2 (c), and 6×2 (d) double chains. Blue arrows indicate the direction of their dipole moments