Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Nitrogen-Phosphorus Codoped Carbon Nanotube Sponges for Detecting Volatile Organic Compounds: Experimental and DFT-Calculations

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Figure S1: Armando D. Martínez-Iniesta et al.

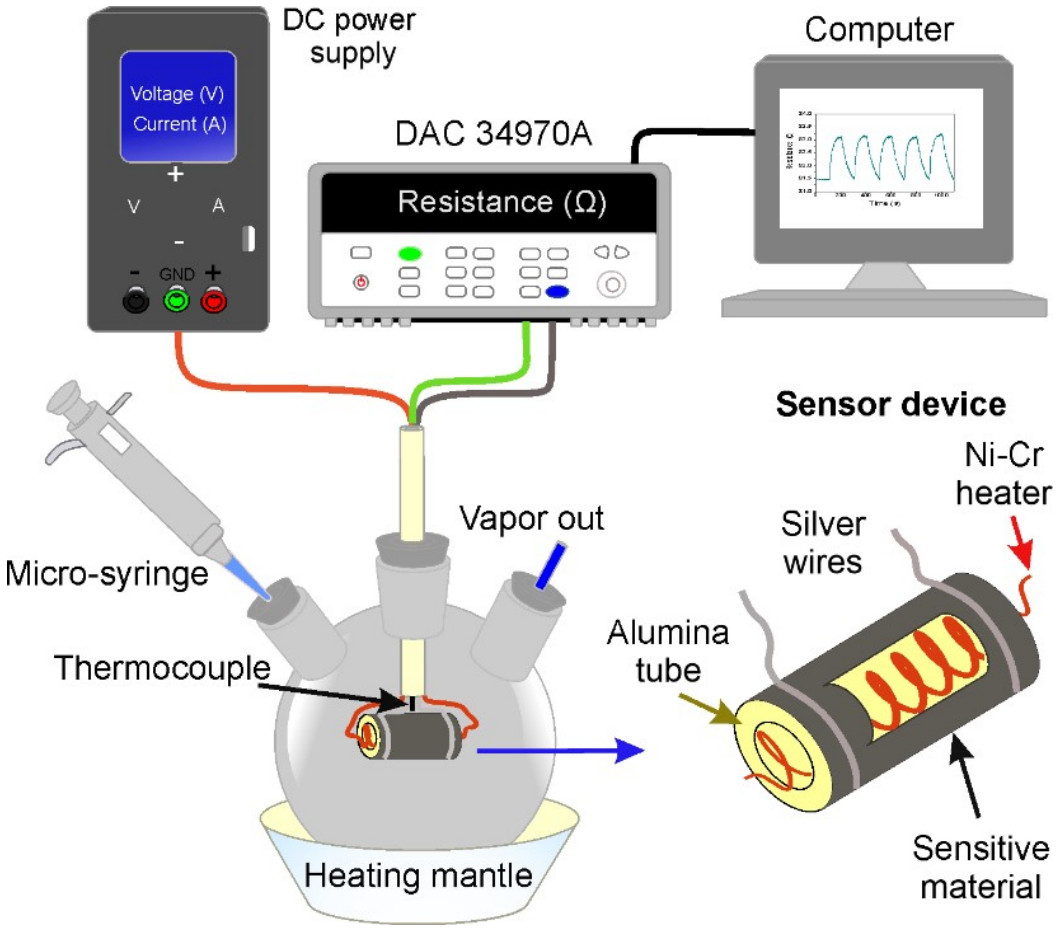

Figure S1: Schematic illustration of the vapor sensing system and the sensor device. The carbon nanotube sponges (NP-CNTSs) are used as sensitive materials in this study. Acetone, cyclohexane, ethanol, isopropanol, and methanol gas vapors were selected to assess the sensor performance. A Ni-Cr heating wire controls the sensor device temperature by tuning the voltage. The sensing measurements were carried out at a relative humidity of 30%.

Figure S2: Armando D. Martínez-Iniesta et al.

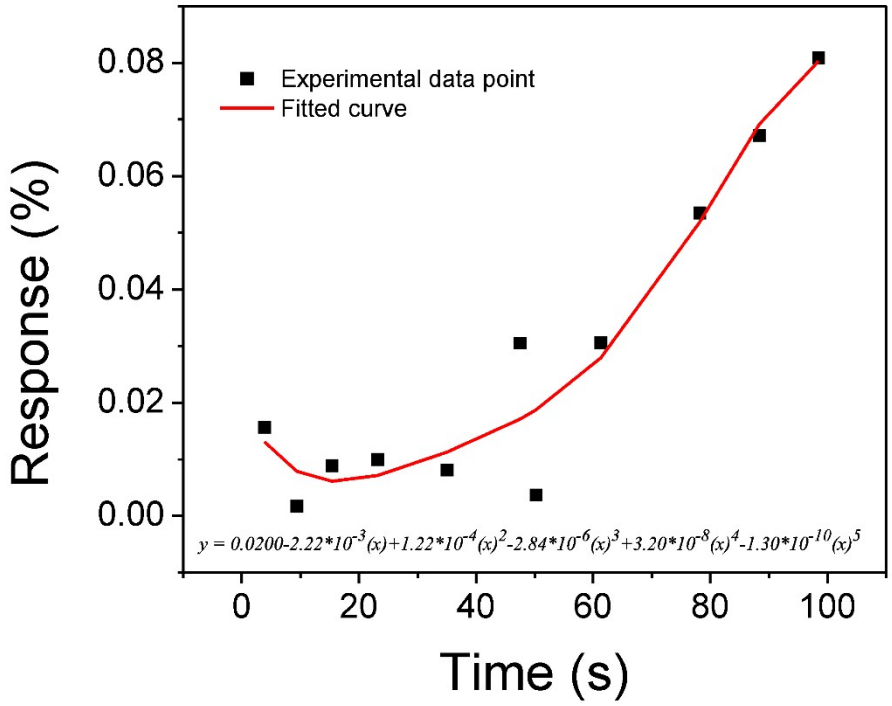

Figure S2: Eleven data points of the response signal in air fitted to the 5th order polynomial.

Figure S3: Armando D. Martínez-Iniesta et al.

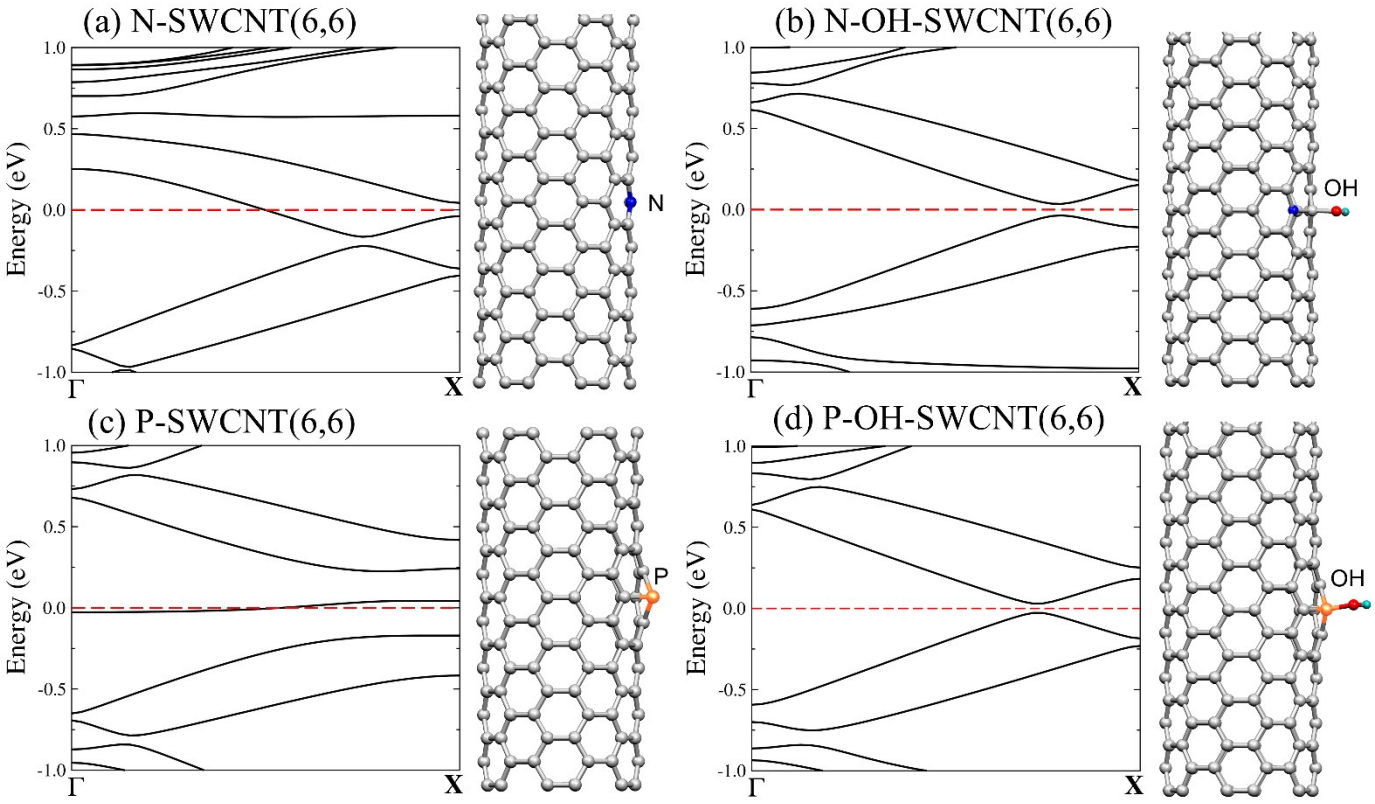

Figure S3: Band structure and optimized structure of P- and N-doped and functionalized SWCNT(6,6) . **(a)** N-SWCNT(6,6), **(b)** N-OH-SWCNT(6,6), **(c)** P-SWCNT(6,6), and **(d)** P-OH-SWCNT(6,6). In all cases, the Fermi level was shifted to zero represented by the dashed line.

Figure S4: Armando D. Martínez-Iniesta et al.

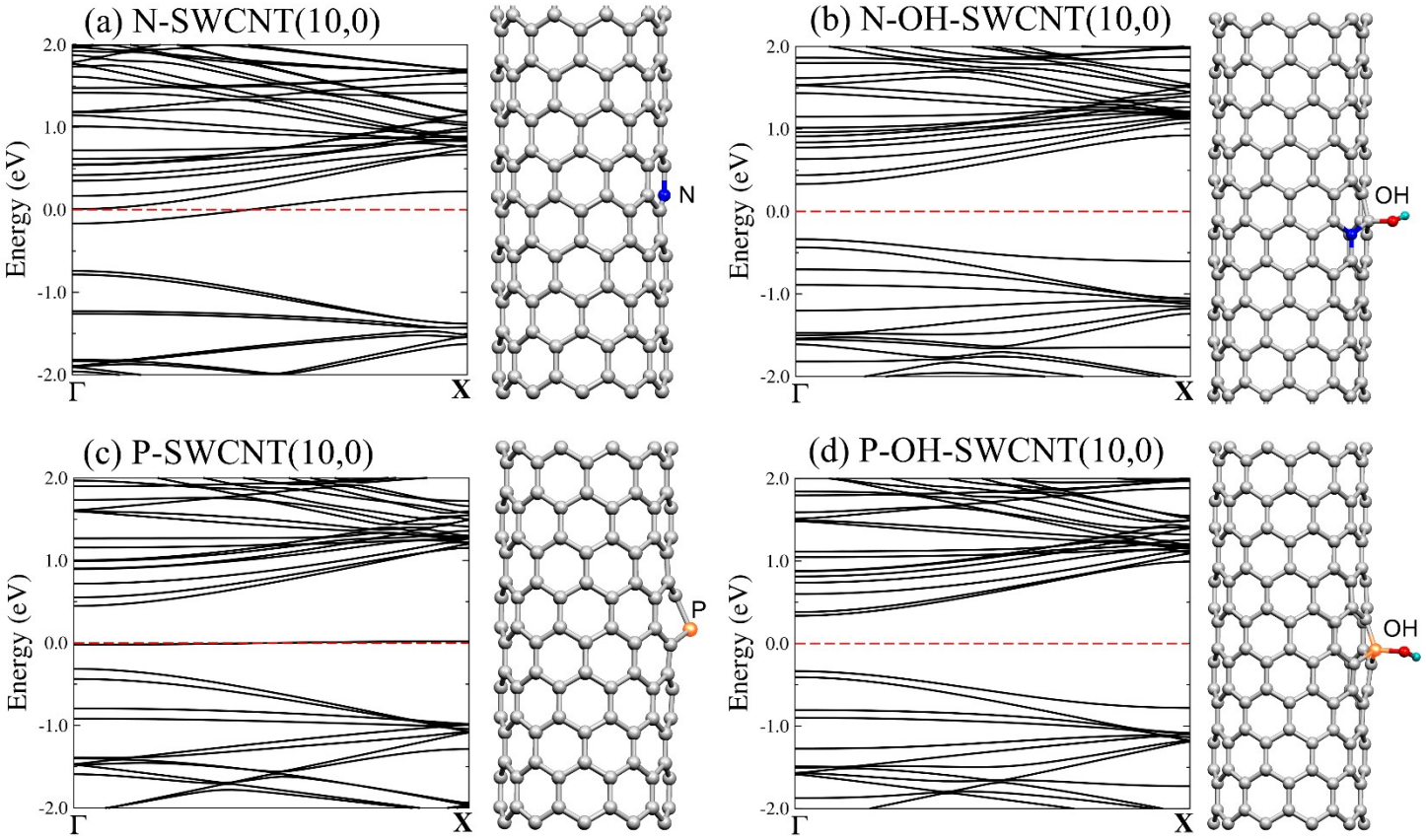

Figure S4: Band structure and optimized structure of P- and N-doped and functionalized SWCNT(10,0) . **(a)** N-SWCNT(10,0), **(b)** N-OH-SWCNT(10,0), **(c)** P-SWCNT(10,10), and **(d)** P-OH-SWCNT(10,0). In all cases, the Fermi level was shifted to zero represented by the dashed line.

Figure S5: Armando D. Martínez-Iniesta et al.

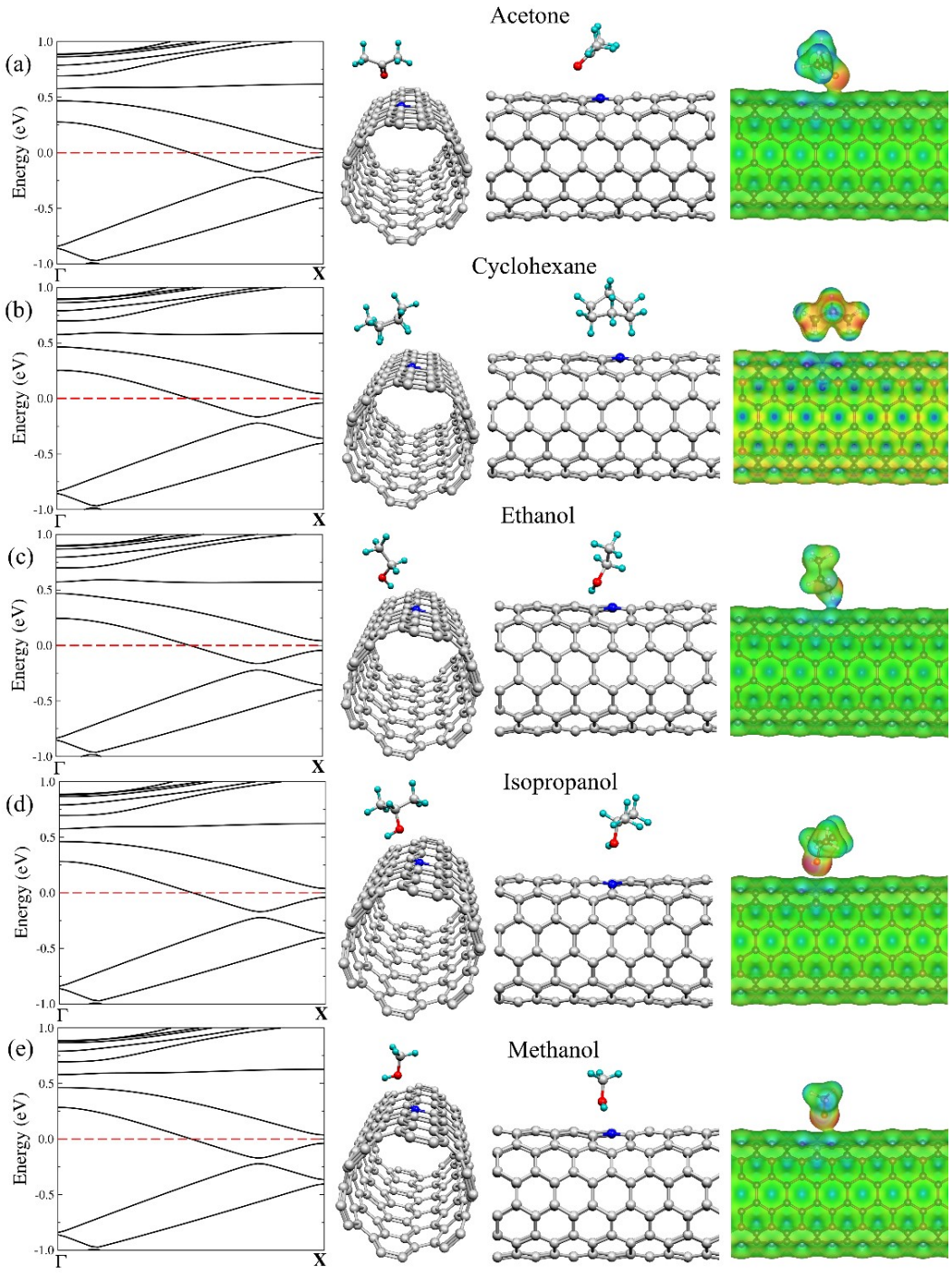

Figure S5: : Band structure, optimized structures, and electrostatic potential surface calculations of N-SWCNT(6,6) interacting with **(a)** acetone, **(b)** cyclohexane, **(c)** ethanol, **(d)** isopropanol, and **(e)** methanol molecules.

Figure S6: Armando D. Martínez-Iniesta et al.

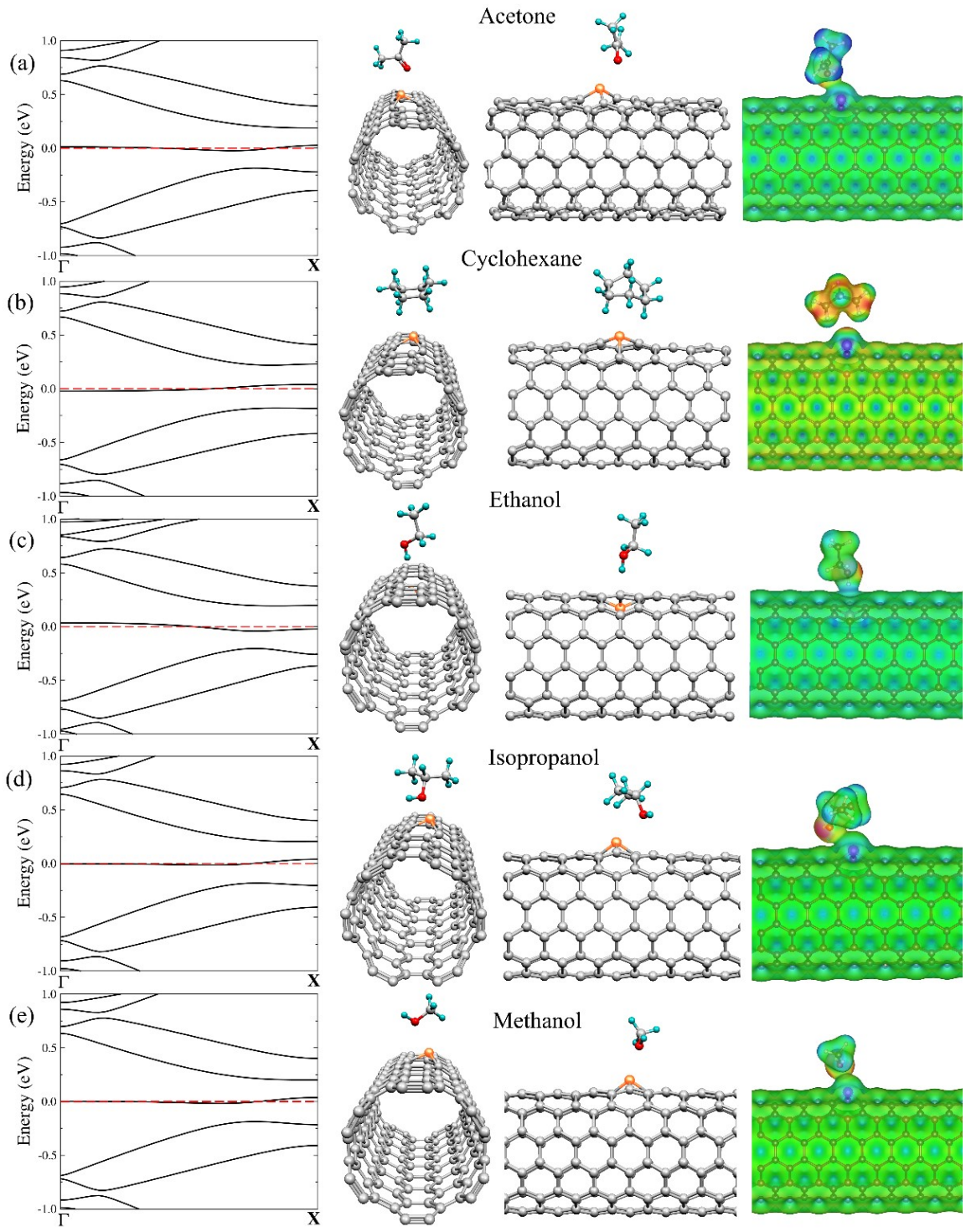

Figure S6: Band structure, optimized structures, and electrostatic potential surface calculations of P-SWCNT(6,6) interacting with **(a)** acetone, **(b)** cyclohexane, **(c)** ethanol, **(d)** isopropanol, and **(e)** methanol molecules.

Figure S7: Armando D. Martínez-Iniesta et al.

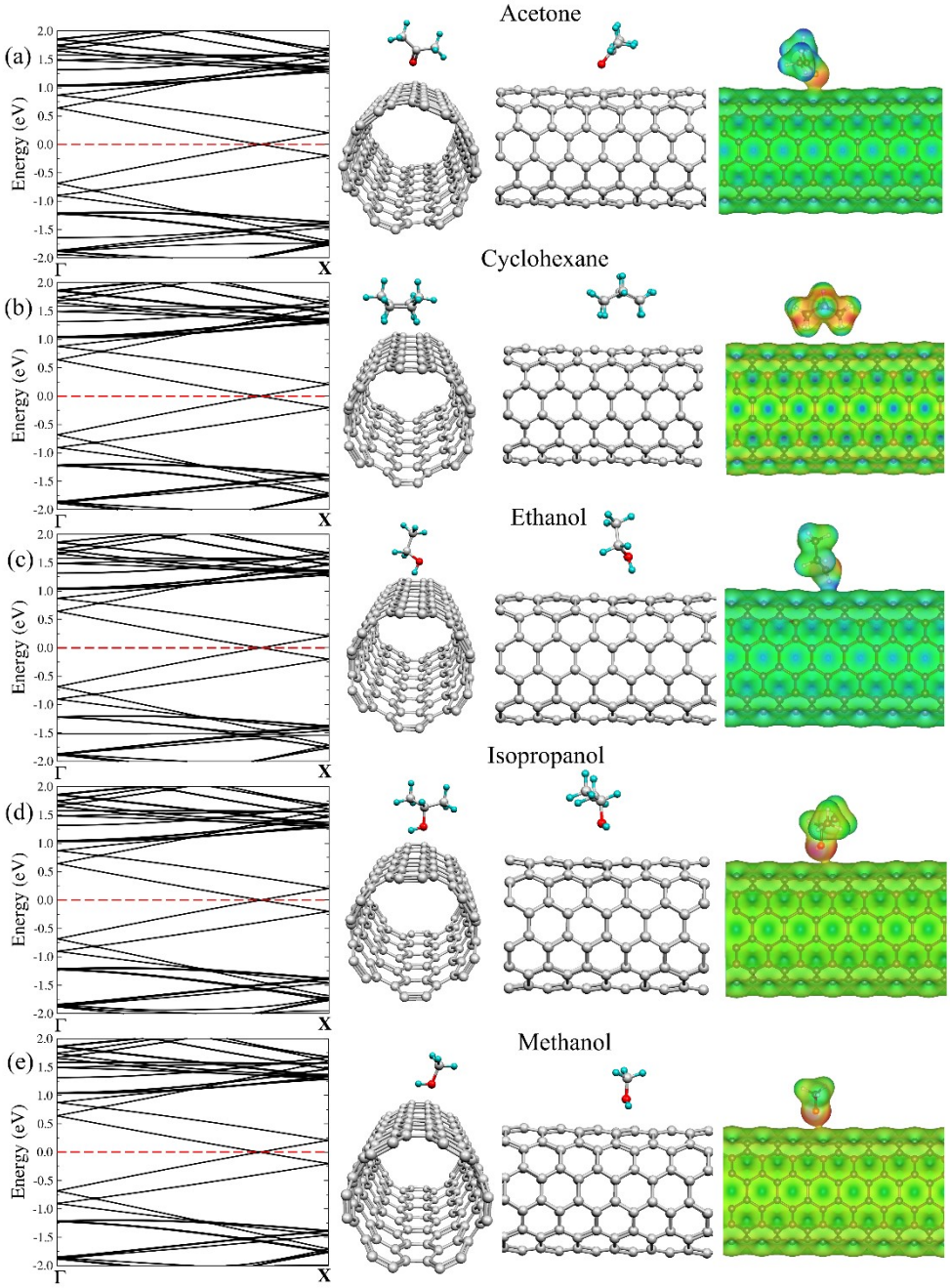

Figure S7: Band structure, optimized structures, and electrostatic potential surface calculations of pristine SWCNT(6,6) interacting with **(a)** acetone, **(b)** cyclohexane, **(c)** ethanol, **(d)** isopropanol, and **(e)** methanol molecules.

Figure S8: Armando D. Martínez-Iniesta et al.

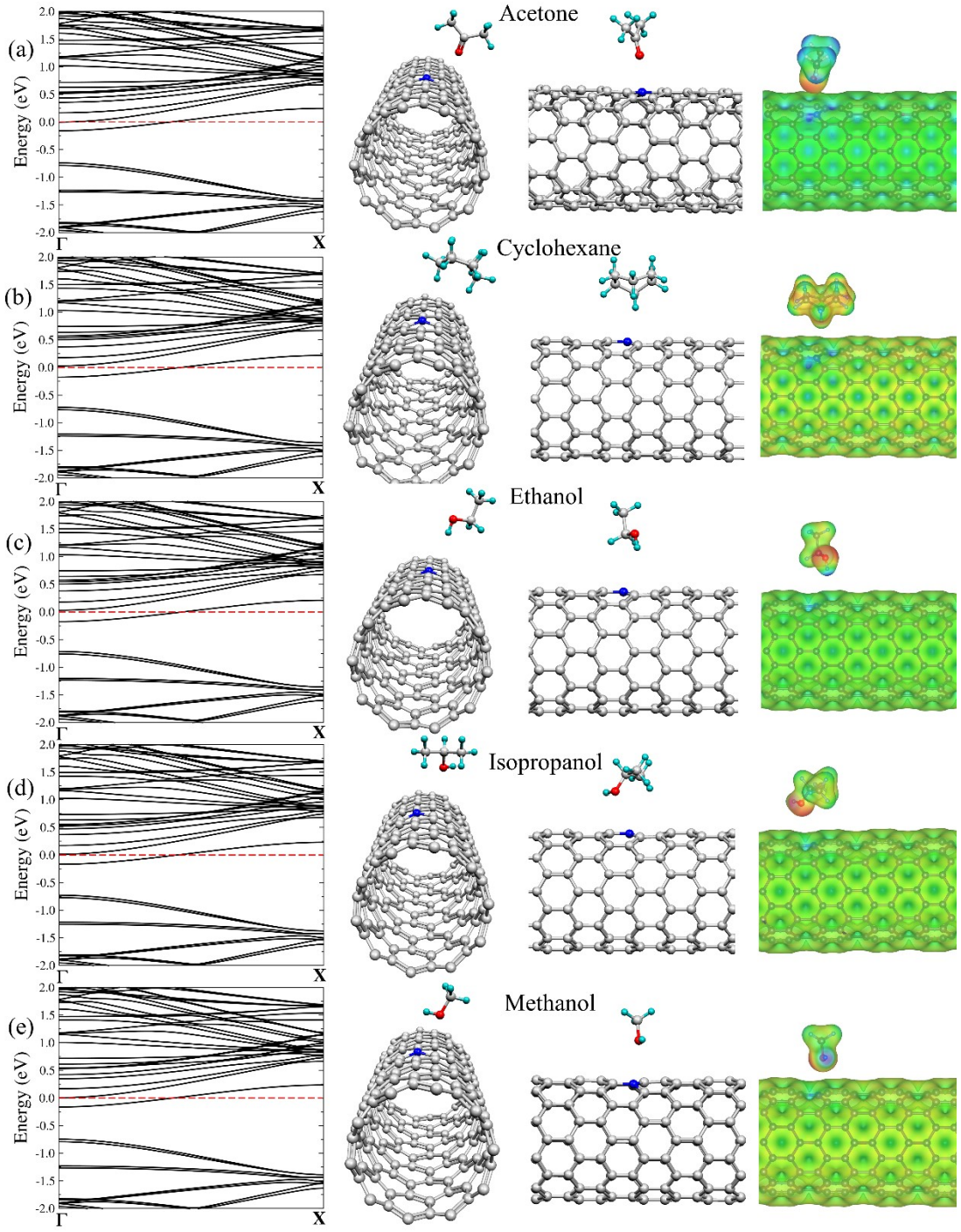

Figure S8: Band structure, optimized structures, and electrostatic potential surface calculations of N-SWCNT(10,0) interacting with **(a)** acetone, **(b)** cyclohexane, **(c)** ethanol, **(d)** isopropanol, and **(e)** methanol molecules.

Figure S9: Armando D. Martínez-Iniesta et al.

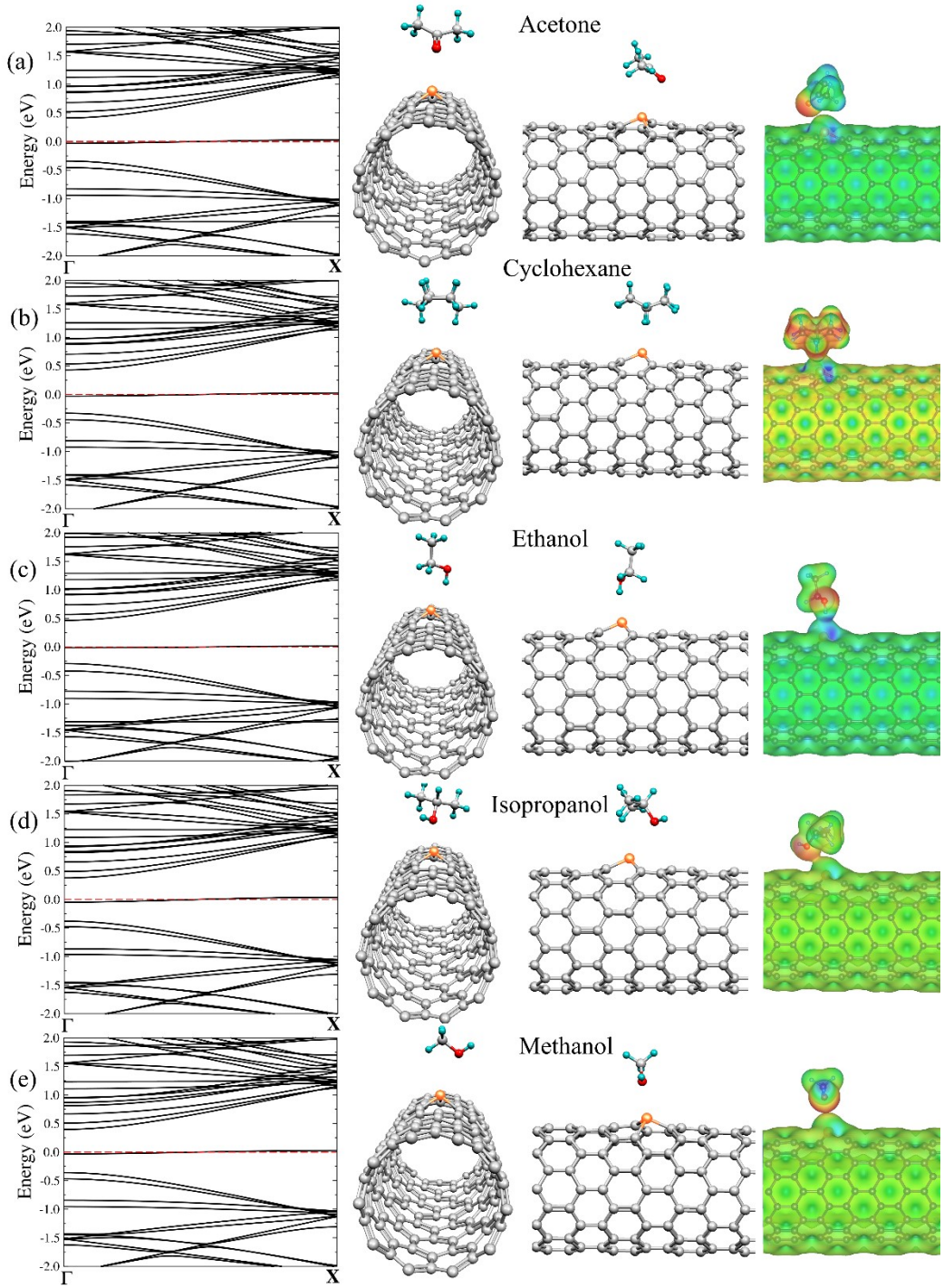

Figure S9: Band structure, optimized structures, and electrostatic potential surface calculations of P-SWCNT(10,0) interacting with **(a)** acetone, **(b)** cyclohexane, **(c)** ethanol, **(d)** isopropanol, and **(e)** methanol molecules.

Figure S10: Armando D. Martínez-Iniesta et al.

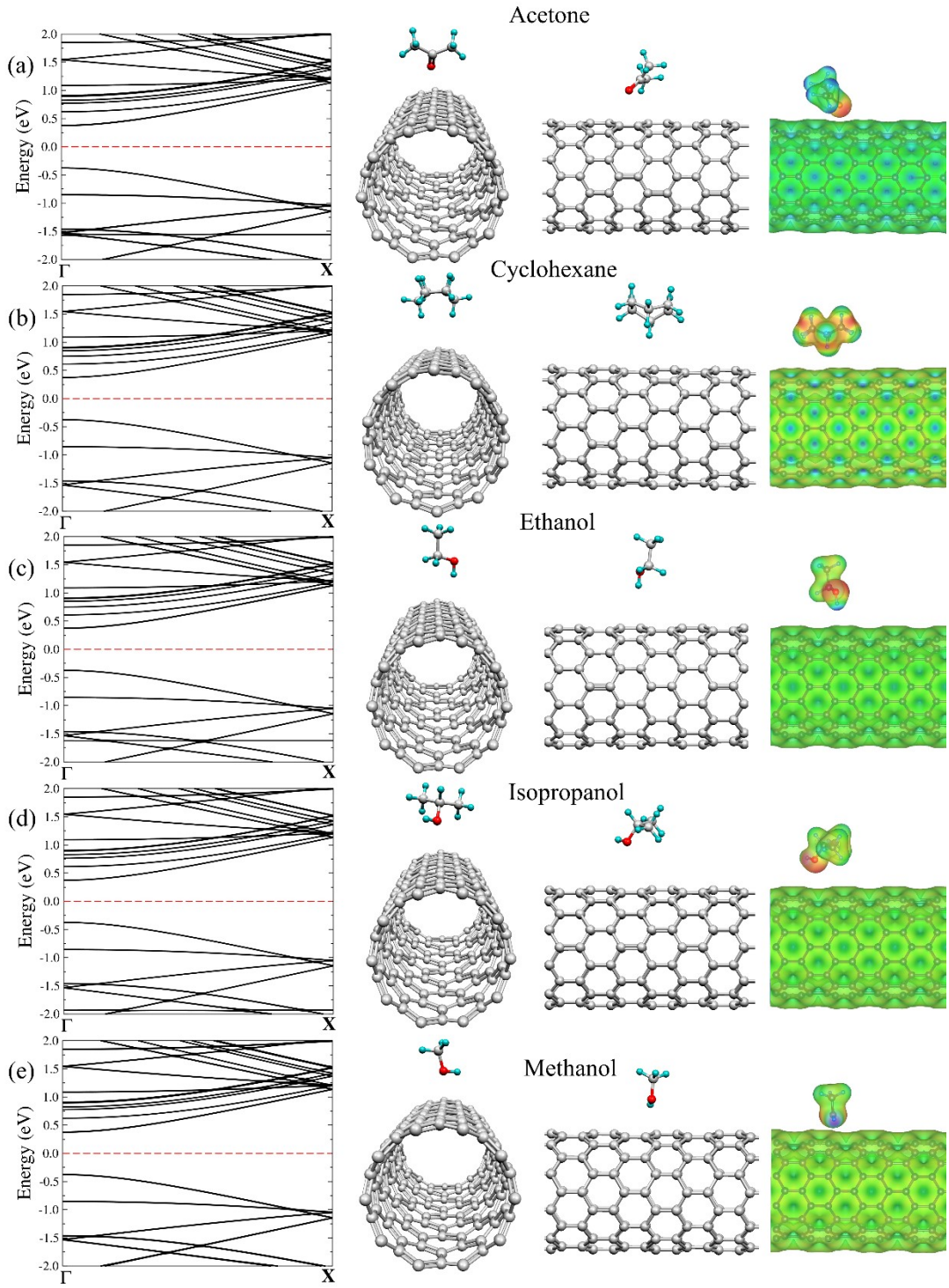

Figure S10: Band structure, optimized structures, and electrostatic potential surface calculations of pristine SWCNT(10,0) interacting with **(a)** acetone, **(b)** cyclohexane, **(c)** ethanol, **(d)** isopropanol, and **(e)** methanol molecules.

Molecule	N-SWCNTs	P-SWCNTs	NP-SWCNTs	NP-OH-SWCNTs	SWCNT
SWCNT(6,6)					
Acetone	0.10660	0.16960	0.47949	0.02743	0.19814
Cyclohexane	-0.00214	0.02258	0.03332	-0.05438	0.07658
Ethanol	0.16091	0.05466	-0.02267	-0.09798	0.14956
Isopropanol	0.08713	0.15245	0.13028	0.21614	0.19820
Methanol	0.09061	0.16573	0.11148	-0.01801	0.14582
SWCNT(10,0)					
Acetone	-0.02961	0.00965	0.04131	0.03720	0.04738
Cyclohexane	-0.01820	0.05918	0.08272	-0.01299	-0.01876
Ethanol	-0.01393	-0.03174	-0.04131	-0.01968	-0.02937
Isopropanol	-0.04810	0.03657	0.10938	-0.12570	-0.02249
Methanol	0.00746	0.01067	0.03923	-0.19570	0.04599

Table S1: Armando D. Martínez-Iniesta et al.

Table S1: GGA-PBE calculations of adsorption energy (E^{cp}_{int}) in eV units for gas molecules placed on the surface of single walled carbon nanotubes (SWCNTs). Results for nitrogen-doped SWCNTs (N-SWCNTs), phosphorus-doped SWCNTs (P-SWCNTs), nitrogen-phosphorus-codoped SWCNTs (NP-SWCNTs), OH-functionalization of NP-SWCNTs (NP-OH-SWCNTs), and pristine SWCNTs. Negative adsorption energy value indicates a stable configuration and exothermic adsorption.