Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Physisorption vs Chemisorption of Probe Molecules on Boron Nitride Nanomaterials. Effect of Surface Curvature

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Table S1. Energy difference (ΔE, kJ mol^{-1}) of different (n,0) carbon and boron nitride nanotubes (CNT and BNNT, respectively) with respect to the corresponding single sheets. For CNTs, calculated per couple of C atoms; for BNNTs per B-N pair.

(n,0)	CNT [a]	BNNT
(4,0)	-	102.9
(5,0)	-	64.4
(6,0)	-	44.8
(7,0)	-	32.9
(9,0)	42.2	20.3
(12,0)	19.2	11.9
(15,0)	12.5	8.0
(18,0)	8.8	5.9
(21,0)	6.6	3.9
(24,0)	5.1	3.1

[a] From R. Demichelis et al., J. Phys. Chem. C, 2011, 115, 8876-8885.

Table S2. BSSE-non-corrected (ΔE_{ads}) and corrected (ΔE^{C}_{ads}) computed adsorption energies (in kJ mol^{-1}) for the interaction of H_2O, NH_3, HCOOH, C_6H_6 and CH_4 with (4,0), (6,0), (9,0) and (15,0) BNNTs and a BNNS, at different levels of calculation (L1, L2 and L3).

System	ΔE_{ads}			ΔE^{C}_{ads}
	L1	L2	L3	L3
H_2O/BNNT(4,0)	-59.4	-73.4	-65.7	-53.3
H_2O/BNNT(6,0)	-18.2	-32.2	-25.0	-16.9
H_2O/BNNT(9,0)	-13.3	-27.8	-22.0	-13.7
H_2O/BNNT(15,0)	-11.9	-25.3	-20.9	-12.7
H_2O/BNNS	-11.4	-25.5	-18.8	-11.4
NH_3/BNNT(4,0)	-108.3	-127.4	-122.2	-111.0
NH_3/BNNT(6,0)	-50.3	-70.9	-65.3	-54.5
NH_3/BNNT(9,0)	-16.3	-39.2	-34.2	-23.6
NH_3/BNNT(15,0)	-9.1	-23.5	-19.2	-16.0
NH_3/BNNS	-4.8	-22.1	-18.4	-14.7
HCOOH/BNNT(4,0)	-61.7	-89.0	-80.5	-71.2
HCOOH/BNNT(6,0)	-21.9	-43.8	-37.7	-31.8
HCOOH/BNNT(9,0)	-17.1	-39.4	-33.6	-27.0
HCOOH/BNNT(15,0)	-14.3	-37.0	-30.7	-25.3
HCOOH/BNNS	-11.5	-36.9	-30.9	-26.9
C_6H_6/BNNT(4,0)	-2.3	-38.4	-35.7	-30.4
C_6H_6 /BNNT(6,0)	-2.5	-41.8	-37.8	-32.6
C_6H_6/BNNT(9,0)	-1.8	-46.0	-41.5	-36.2
C_6H_6/BNNT(15,0)	-1.4	-49.3	-44.2	-38.9
C_6H_6/BNNS	-2.1	-60.4	-52.9	-48.4
CH_4/BNNT(4,0)	-1.2	-13.4	-12.5	-9.9
CH_4 /BNNT(6,0)	-0.5	-12.7	-12.3	-10.3
CH_4/BNNT(9,0)	-0.3	-13.9	-12.7	-10.7
CH_4/BNNT(15,0)	0.1	-14.4	-13.1	-11.1
CH_4/BNNS	0.0	-17.2	-15.9	-14.0

L1: B3LYP/6-311G(d,p)
L2: B3LYP-D*/6-311G(d,p)
L3: BN nanomaterials at B3LYP-D*/6-311G(d,p) and probe molecules at B3LYP-D*/TZP.

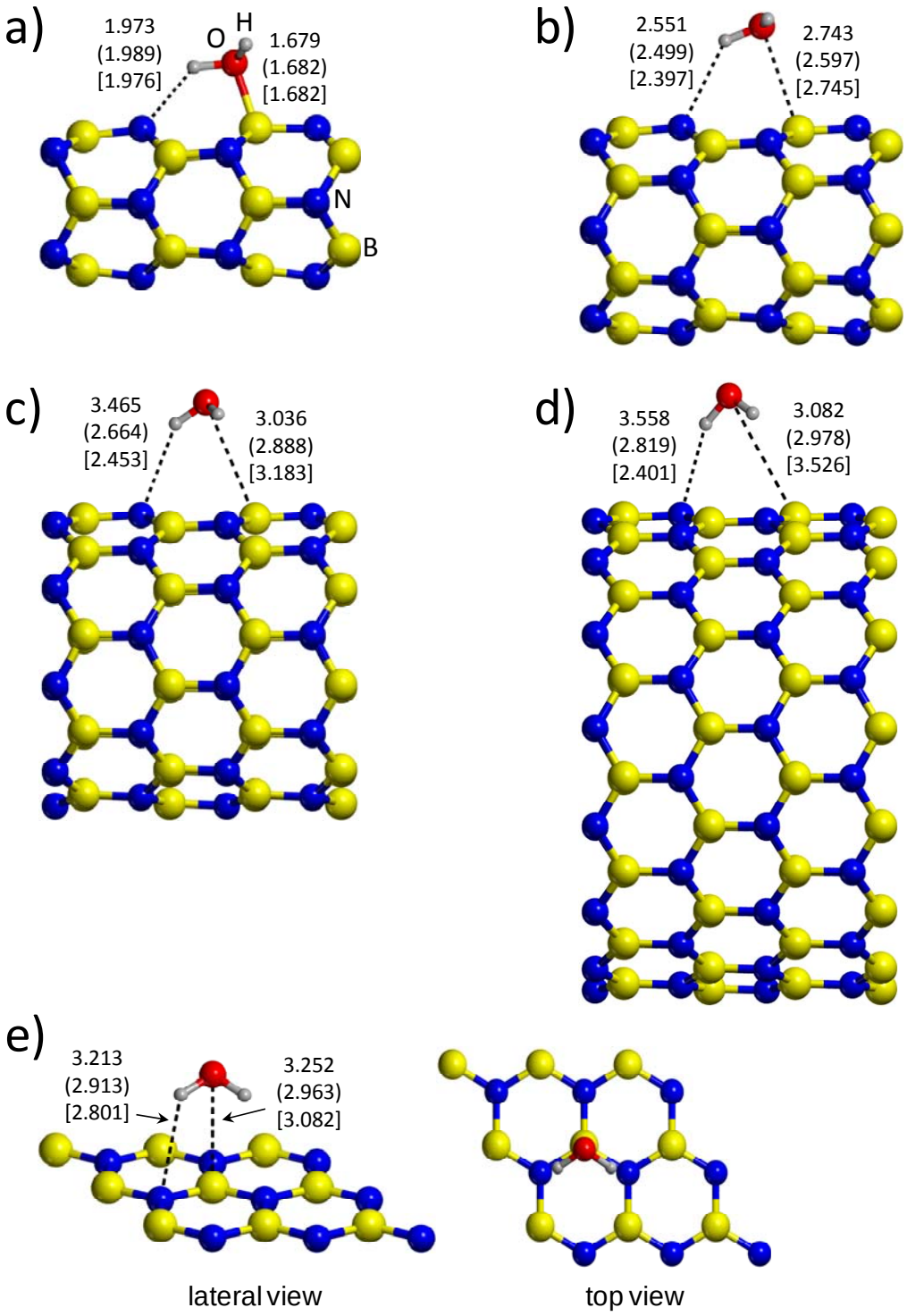

Figure S1. Optimized structures of H_2O interacting with the different BN nanomaterials computed at different levels: bare values at B3LYP/6-311G(d,p); values in parenthesis at B3LYP-D*/6-311G(d,p); values in brackets, the B and N atoms of the BN nanomaterials at B3LYP-D*/6-311G(d,p) and the atoms of H_2O at B3LYP-D* using a TZP basis set from the Ahlrichs and coworkers. Distances in Å.

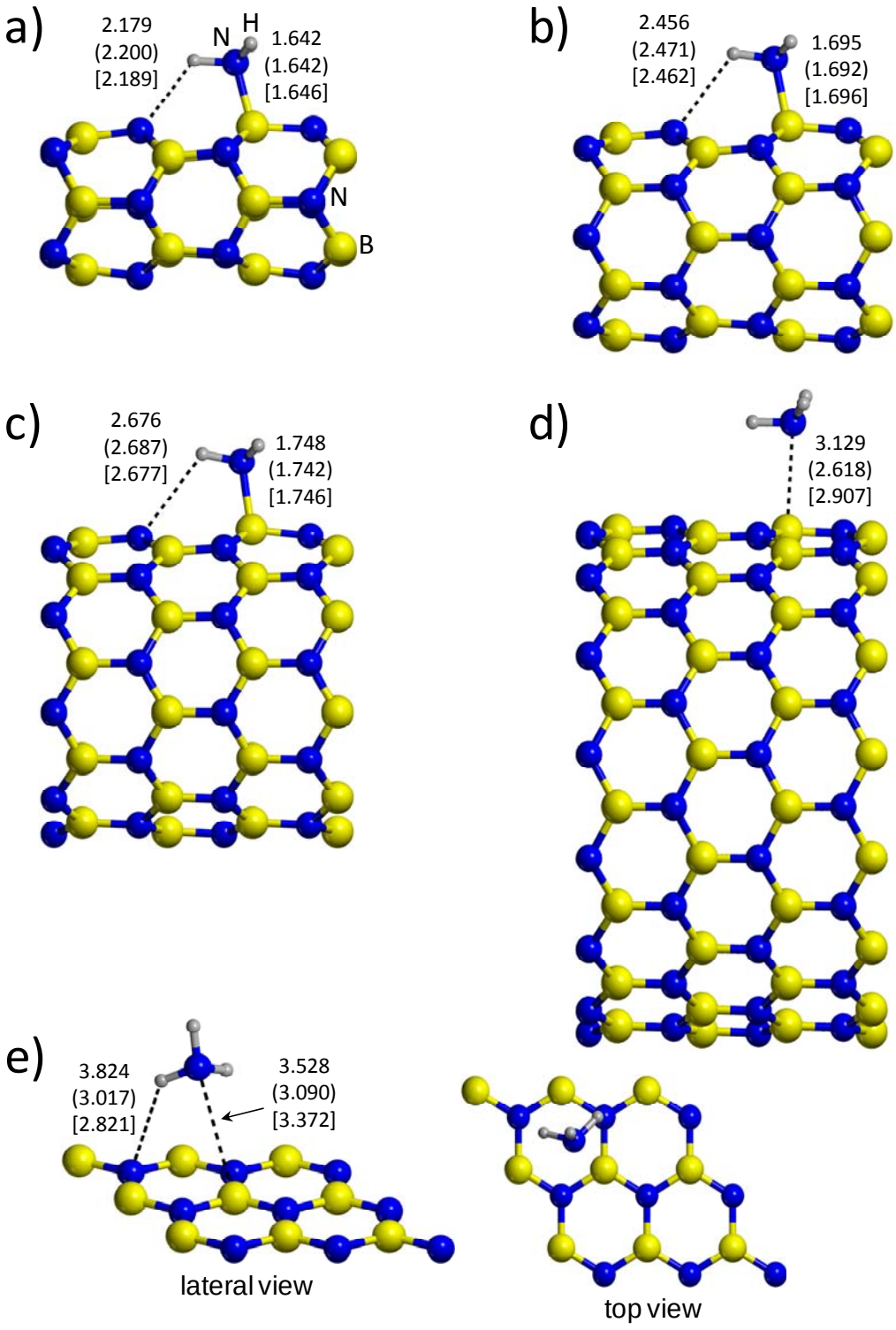

Figure S2. Optimized structures of NH_3 interacting with the different BN nanomaterials computed at different levels: bare values at B3LYP/6-311G(d,p); values in parenthesis at B3LYP-D*/6-311G(d,p); values in brackets, the B and N atoms of the BN nanomaterials at B3LYP-D*/6-311G(d,p) and the atoms of NH_3 at B3LYP-D* using a TZP basis set from the Ahlrichs and coworkers. Distances in Å.

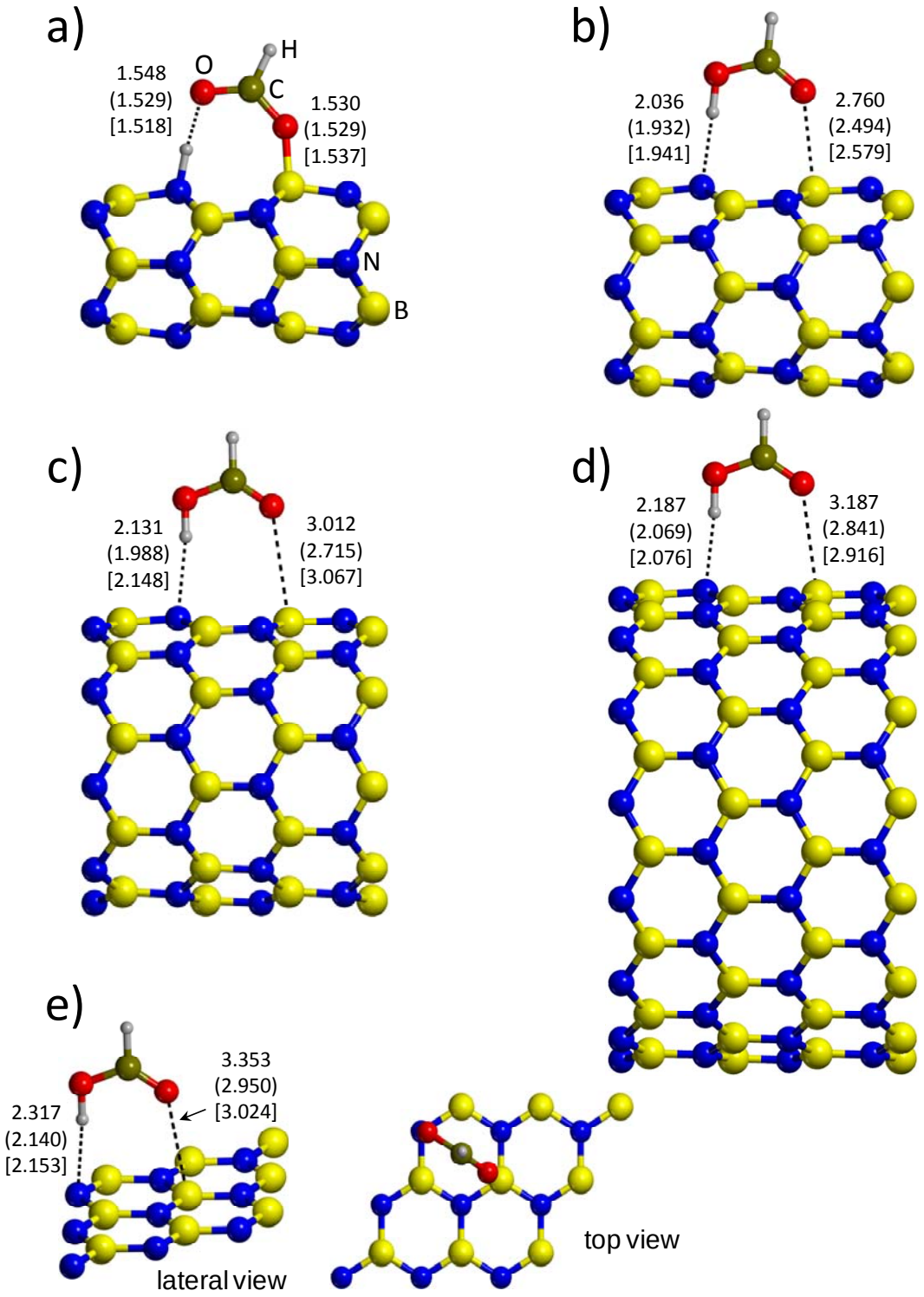

Figure S3. Optimized structures of HCOOH interacting with the different BN nanomaterials computed at different levels: bare values at B3LYP/6-311G(d,p); values in parenthesis at B3LYP-D*/6-311G(d,p); values in brackets, the B and N atoms of the BN nanomaterials at B3LYP-D*/6-311G(d,p) and the atoms of HCOOH at B3LYP-D* using a TZP basis set from the Ahlrichs and coworkers. Distances in Å.

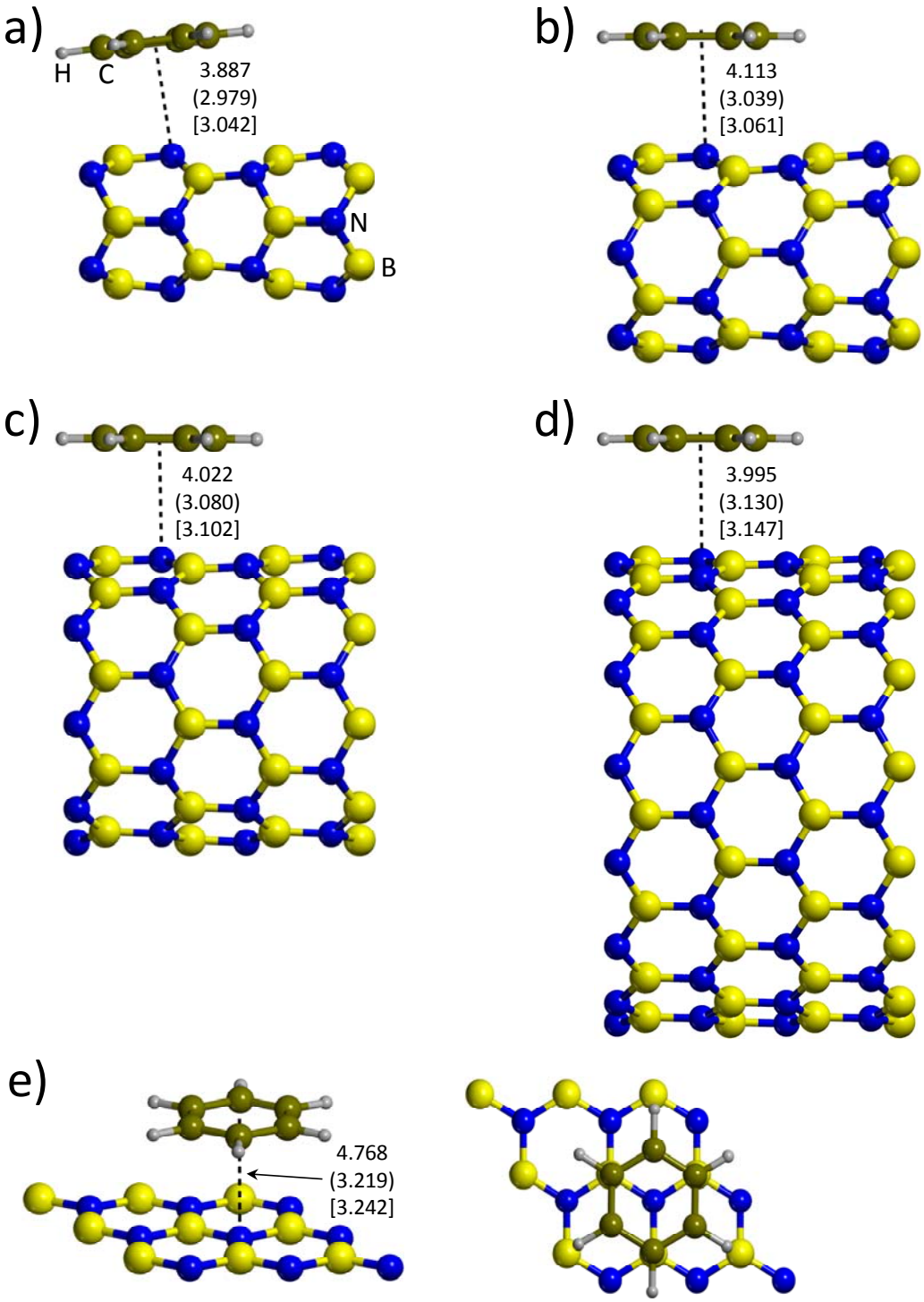

Figure S4. Optimized structures of C_6H_6 interacting with the different BN nanomaterials computed at different levels: bare values at B3LYP/6-311G(d,p); values in parenthesis at B3LYP-D*/6-311G(d,p); values in brackets, the B and N atoms of the BN nanomaterials at B3LYP-D*/6-311G(d,p) and the atoms of C_6H_6 at B3LYP-D* using a TZP basis set from the Ahlrichs and coworkers. Distances in Å.

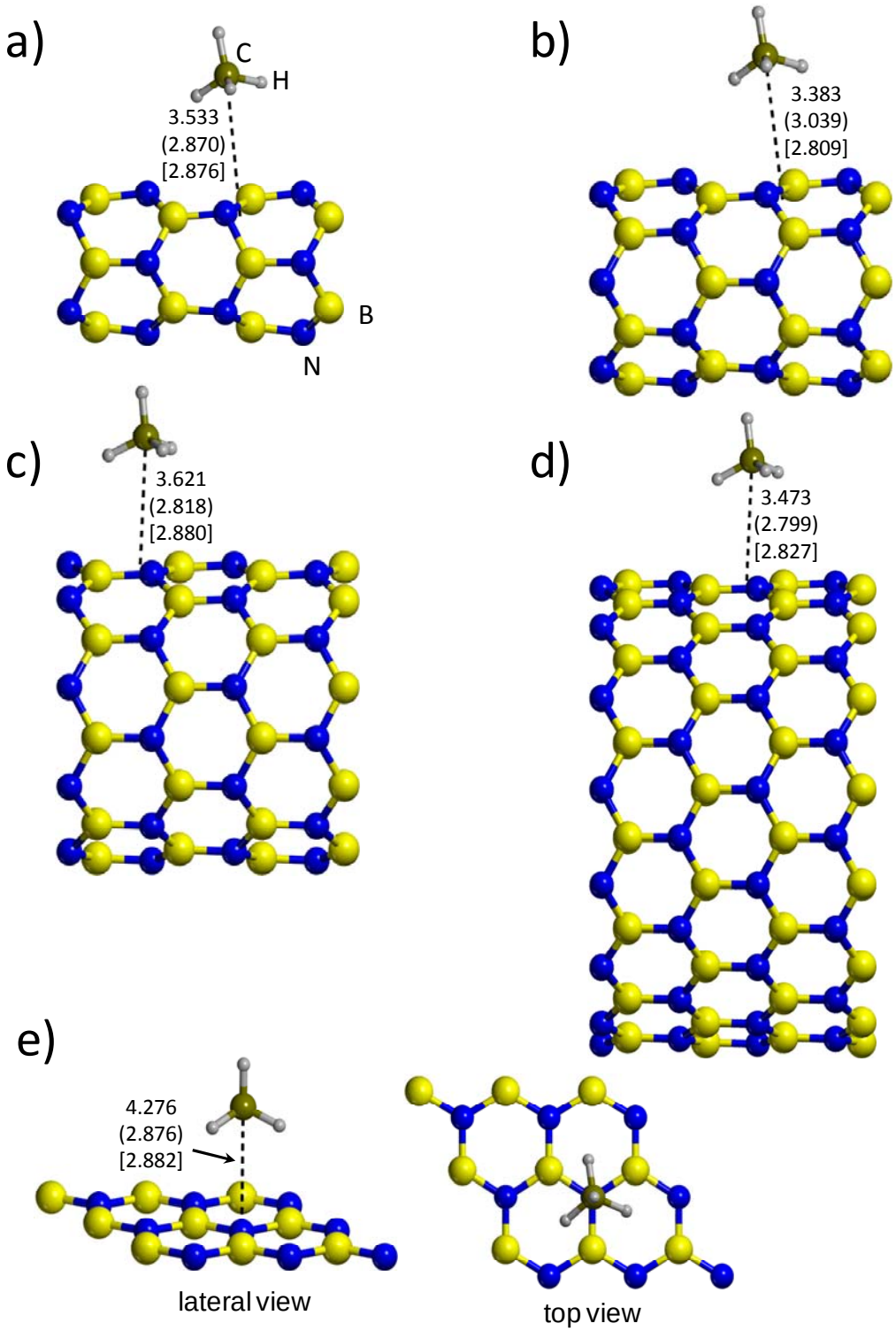

Figure S5. Optimized structures of CH_4 interacting with the different BN nanomaterials computed at different levels: bare values at B3LYP/6-311G(d,p); values in parenthesis at B3LYP-D*/6-311G(d,p); values in brackets, the B and N atoms of the BN nanomaterials at B3LYP-D*/6-311G(d,p) and the atoms of CH_4 at B3LYP-D* using a TZP basis set from the Ahlrichs and coworkers. Distances in Å.