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The VN_3H Defect in Diamond: A Quantum-Mechanical Characterization. Supplemental Material

Francesco Silvio Gentile,[1] Simone Salustro,[1] Mauro Causà,[2] Alessandro Erba,[3] Philippe Carbonniére,[4] and Roberto Dovesi[1]

[1]*Dipartimento di Chimica, Università di Torino and NIS - Nanostructured Interfaces and Surfaces - Centre of Excellence, Via Giuria 5, 10125 Torino, Italy*
[2]*Dipartimento di Ingengeria Chimica, dei Materiali e delle Produzioni Industriali, Università degli studi di Napoli Federico II (Nanostructured Interfaces and Surfaces) Centre, Via P. Giuria 5, 10125 Torino, Italy*
[3]*Dipartimento di Chimica, Università di Torino and NIS (Nanostructured Interfaces and Surfaces) Centre, Via P. Giuria 5, 10125 Torino, Italy*
[4]*Equipe de Chimie Physique, IPREM UMR5254, Université de Pau et des Pays de l'Adour, 64000 Pau (France)*

I. HOMOLYTIC FISSION OF THE C-H BOND.

Table S1: Energy required for the homolytic dehydrogenation (ΔE_H) of methane CH_4, ethane C_2H_6, propane C_3H_8 and isobutane C_4H_{10}. The energy has been evaluated using the B3LYP functional. Indices *t*, *s* and *p* characterize the carbon atom on which the radical is located: ternary, meaning that the carbon atom is linked to three other carbon atoms, secondary and primary. In the lowest part of the Table the effect of the functional is reported in the C_2H_6 case. Total energies in hartree, ΔE_H and in eV.

R group	H_2	R·	R-H	ΔE_H
H·	-1.16872	- 4.968621	-	+2.381
CH_3·	-1.16872	-39.766981	-40.44889	+2.655
C_2H_5· (*p*)	-1.16872	-79.023618	-79.69719	+2.428
C_3H_7·(*p*)	-1.16872	-118.273995	-118.94782	+2.434
C_4H_9·(*p*)	-1.16872	-157.52555	-158.19980	+2.447
C_3H_7·(*s*)	-1.16872	-118.281550	-118.94782	+2.229
C_4H_9·(*t*)	-1.16872	-157.53977	-158.19980	+2.060

Method	H_2	C_2H_5·	C_2H_6	ΔE_H
B3LYP	-1.16872	-79.023618	-79.69719	-2.428
PBE0	-1.16389	-78.979524	-79.65307	-2.493
HSE06	-1.16357	-78.977171	-79.65050	-2.491
PBE	-1.16198	-78.959341	-79.63236	-2.504
LDA	-1.13325	-78.289382	-78.96125	-2.864