**Supplementary Materials for**

**Theoretical study on the interaction of Heptafluoro-iso-butyronitrile decomposition products with Al (1 1 1)**

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Table S1 Parameters of C2F5CN, CF3CN, COF2 and CF4 adsorbed on Al (1 1 1) with different initial adsorption sites

|  |  |  |
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| Initial structure | Adsorption energy *Ead*(eV) | Total charge transfer *Qt*(e) |
| C2F5CN-N-Top | -0.6289 | -0.219 |
| C2F5CN-N-Bridge | -1.4289 | -0.602 |
| C2F5CN-N-Fcc | -0.6273 | -0.214 |
| C2F5CN-N-Hcp | -0.3782 | 0.004 |
| C2F5CN-CF2-Top | -0.2852 | -0.008 |
| C2F5CN-CF2-Bridge | -0.2852 | -0.011 |
| C2F5CN-CF2-Fcc | -0.2944 | -0.01 |
| C2F5CN-CF2-Hcp | -1.4338 | -0.639 |
| C2F5CN-CF3-Top | -0.2686 | -0.006 |
| C2F5CN-CF3-Bridge | -0.2690 | -0.004 |
| C2F5CN-CF3-Fcc | -0.2760 | 0 |
| C2F5CN-CF3-Hcp | -0.2777 | 0.001 |
| CF3CN-N-Top | -0.4566 | -0.032 |
| CF3CN-N-Bridge | -0.1760 | 0.031 |
| CF3CN-N-Fcc | -0.1738 | 0.026 |
| CF3CN-N-Hcp | -0.4525 | -0.195 |
| CF3CN-C-Top | -1.3492 | -0.6 |
| CF3CN-C-Bridge | -0.2827 | -0.05 |
| CF3CN-C-Fcc | -0.4546 | -0.034 |
| CF3CN-C-Hcp | -1.4103 | -0.612 |
| CF3CN-CF3-Top | -0.1787 | 0.014 |
| CF3CN-CF3-Bridge | -0.1833 | 0.014 |
| CF3CN-CF3-Fcc | -0.1829 | 0.013 |
| CF3CN-CF3-Hcp | -0.1833 | 0.013 |
| COF2-O-Top | -0.1804 | 0.031 |
| COF2-O-Bridge | -0.1187 | 0.027 |
| COF2-O-Fcc | -0.1181 | 0.025 |
| COF2-O-Hcp | -0.1133 | 0.023 |
| COF2-C-Top | -0.1342 | 0.011 |
| COF2-C-Bridge | -0.1364 | 0.009 |
| COF2-C-Fcc | -0.1267 | 0.009 |
| COF2-C-Hcp | -0.1306 | 0.008 |
| COF2-C-parallel-Top | -0.2097 | 0.018 |
| COF2-C-parallel-Bridge | -0.2057 | 0.018 |
| COF2-C-parallel-Fcc | -0.2083 | 0.024 |
| COF2-C-parallel-Hcp | -0.2118 | 0.022 |
| CF4-F-Top | -0.1512 | 0.015 |
| CF4-F-Bridge | -0.0862 | 0.009 |
| CF4-F-Fcc | -0.0877 | 0.008 |
| CF4-F-Hcp | -0.0872 | 0.008 |
| CF4-CF3-Top | -0.1390 | 0.018 |
| CF4-CF3-Bridge | -0.1470 | 0.017 |
| CF4-CF3-Fcc | -0.1503 | 0.014 |
| CF4-CF3-Hcp | -0.1515 | 0.015 |
| CF4-CF2-Top | -0.1247 | 0.014 |
| CF4-CF2-Bridge | -0.1216 | 0.011 |
| CF4-CF2-Fcc | -0.1528 | 0.015 |
| CF4-CF2-Hcp | -0.1503 | 0.015 |