Electronic Supplementary Information

High Resolution Noncontact Atomic Force Microscopy Imaging with Oxygen-Terminated Copper Tips at 78 K

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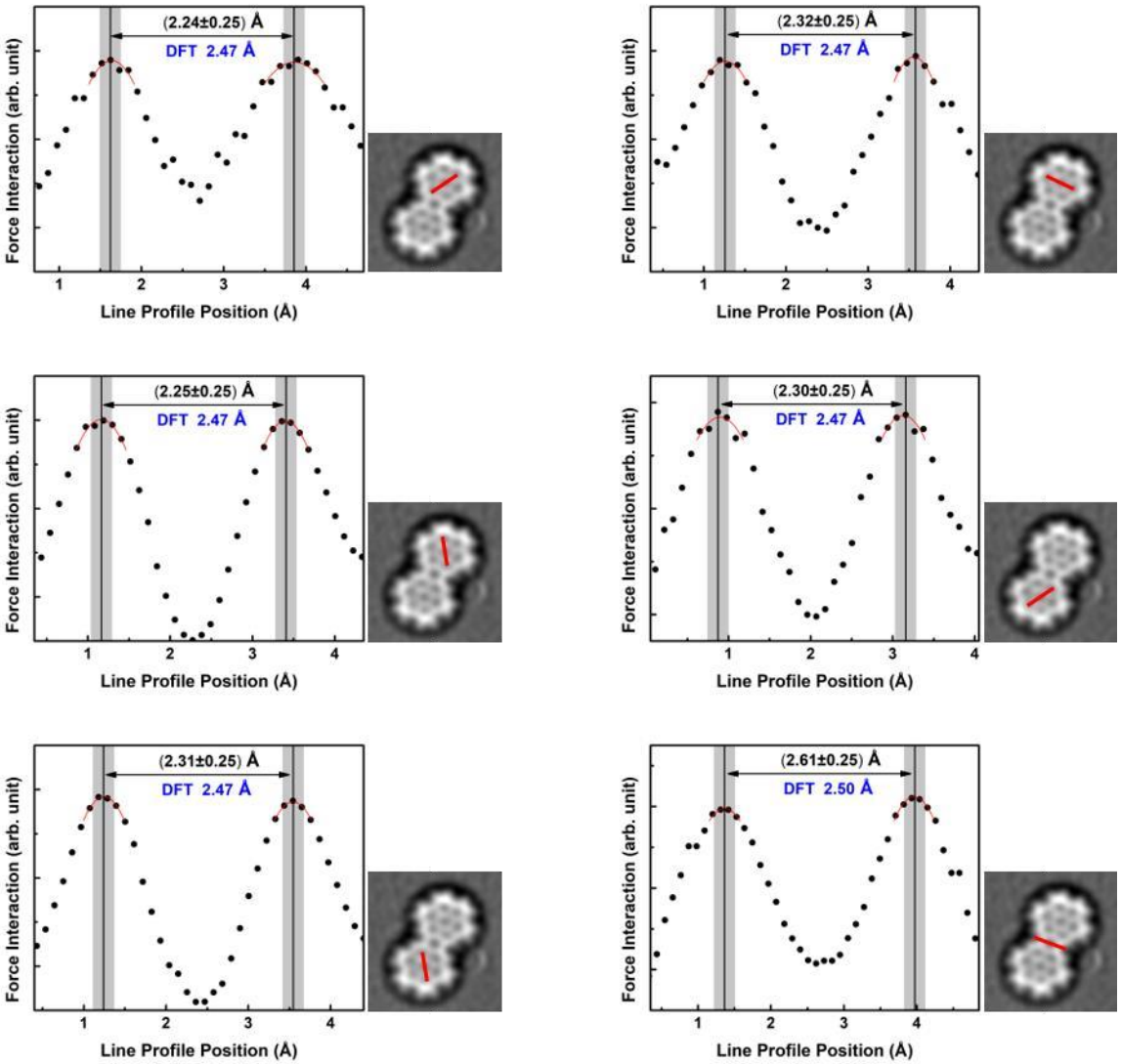

Fig. S1 Line profiles taken from the DCLN molecule.

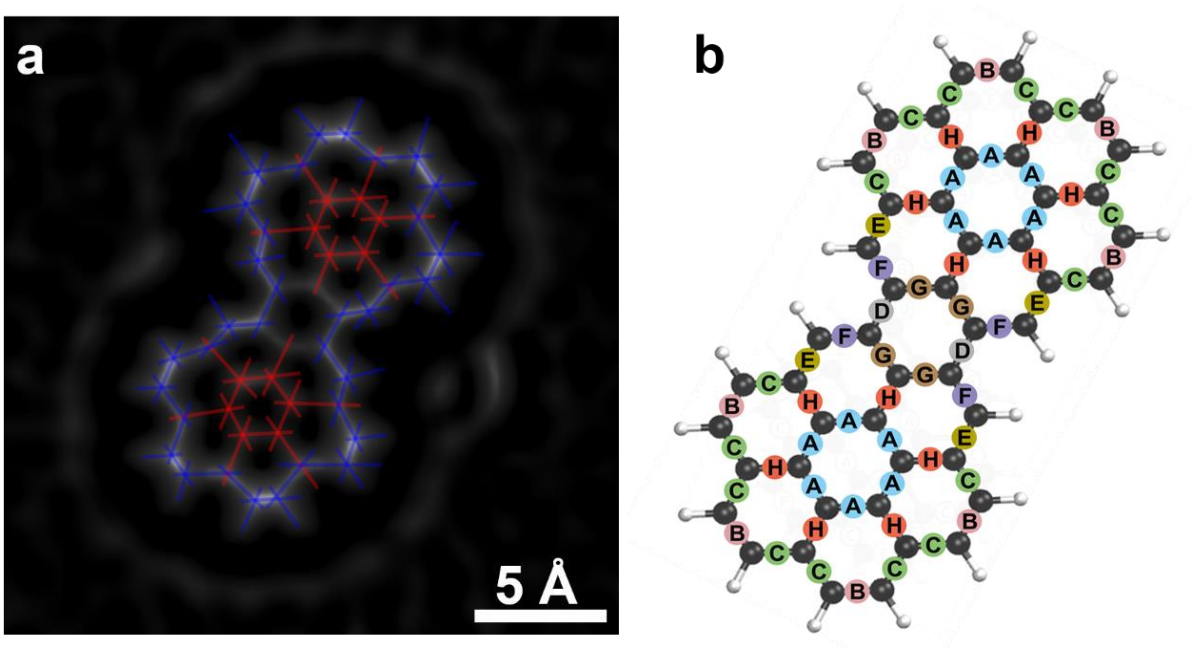

Fig. S2 (a) Fitted straight lines to measure the bond lengths on SD filtered image, (b) Each bond considered in the groups given in the manuscript marked accordingly on the model of DCLN molecule.

Computational Details:

The geometry optimization of the DCLN molecule in the gas phase was performed using the B3LYP functional [1] together with the TZVPP basis set [2] as implemented in the TURBOMOLE V6.3 program package[3]. In addition, the RI approximation[4] and the D3-dispersion correction was applied.[5,6]

[1] Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. J. Phys. Chem. 1994, 98, 11623−11627.

[2] F. Weigend and R. Ahlrichs; Phys. Chem. Chem. Phys. 7, 3297 (2005).

[3] TURBOMOLE V6.3 2011, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.

[4] K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs; Chem. Phys. Letters 242, 652 (1995).

[5] S. Grimme; J. Antony; S. Ehrlich; H. Krieg. J. Chem. Phys., 132, 154104, (2010).

[6] S. Grimme, S. Ehrlich and L. Goerigk, J. Comput. Chem., 2011, 32,1456–1465.