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

Supplementary Information

A Quinone Based Single-Molecule Switch as Building Block for Molecular Electronics

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Table S1. Cartesian coordinates (in Å) of the undoped and Fe-doped quinone molecule

Undoped quinone molecule					Fe-doped quinone molecule			
C	0.0000	0.0000	0.0000		C	0.0000	0.0000	0.0000
C	0.0000	0.0000	1.4500		C	0.0000	0.0000	1.4578
C	1.1536	-0.0020	2.1561		C	1.2009	-0.0359	2.2061
C	2.4531	-0.0106	1.4995		C	2.5135	-0.1246	1.5806
C	2.4577	0.0219	0.0170		C	2.5143	0.1171	0.1287
C	1.2746	0.0129	-0.6728		C	1.3067	0.2752	-0.5933
H	-0.9658	-0.0018	1.9604		H	-0.9612	-0.0260	1.9774
H	1.1464	-0.0083	3.2492		H	1.1509	-0.0844	3.2974
H	1.2799	0.0253	-1.7656		H	1.3601	0.4189	-1.6762
C	-1.1897	-0.0087	-0.6679		C	-1.1652	0.0331	-0.7259
H	-2.1361	-0.0154	-0.1269		H	-2.1323	-0.0835	-0.2377
H	-1.2321	-0.0088	-1.7578		H	-1.1526	0.1611	-1.8080
N	3.6068	-0.0594	2.0955		N	3.6833	-0.1763	2.1836
H	4.4639	-0.0967	0.1049		H	4.5097	0.2019	0.2179
H	3.4850	-0.0841	3.1164		H	3.5556	-0.2611	3.1991
N	3.7011	0.0868	-0.5453		N	3.7538	0.1239	-0.4660
H	3.8225	-0.1688	-1.5167		H	3.8661	0.6250	-1.3399
					Fe	1.1609	1.6528	0.9926