

# Electronic Supplementary Information to: Endohedral metallofullerenes, $M@C_{60}$ ( $M=Ca, Na, Sr$ ): Selective adsorption and sensing of open-shell $NO_x$ gases

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**Table 1** Net Hirshfeld charge in units of electron charge,  $|e|$ .  $\rho_M$  represents the Hirshfeld charge of the metal dopant before gas adsorption.  $\Delta\rho_M$  represents the change in the Hirshfeld charge of the metal dopant after gas adsorption compared to the net Hirshfeld charge of the metal before the adsorption of the gas molecule.  $\rho_g$  represents the Hirshfeld charge of the gas molecule. (GGA results)

System	$\rho_M$	$\Delta\rho_M$		$\rho_g$	
		NO	NO <sub>2</sub>	NO	NO <sub>2</sub>
C <sub>60</sub>				+0.021	-0.011
Ca@C <sub>60</sub>	+0.756	-0.005	-0.008	+0.015	-0.129
Na@C <sub>60</sub>	+0.376	-0.001	-0.011	+0.035	-0.131
Sr@C <sub>60</sub>	+0.69	-0.011	-0.013	+0.002	-0.129

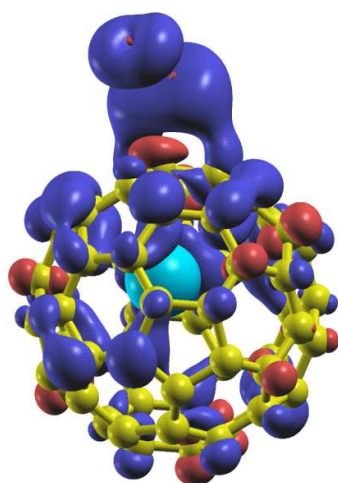
## 1 Cartesian Coordinates

The Cartesian coordinate files for the 32 GGA structures and the 32 VV structures are attached in a separate zipped folder.

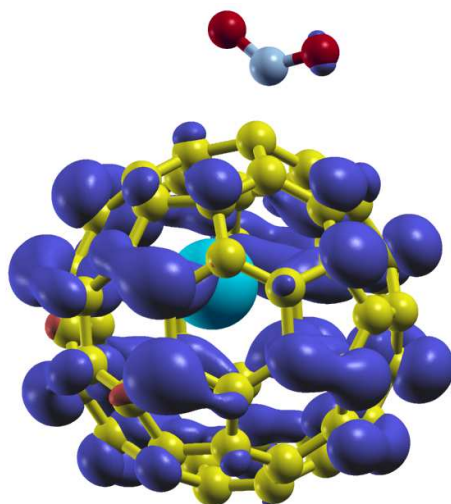
## 2 Spin Density Distribution

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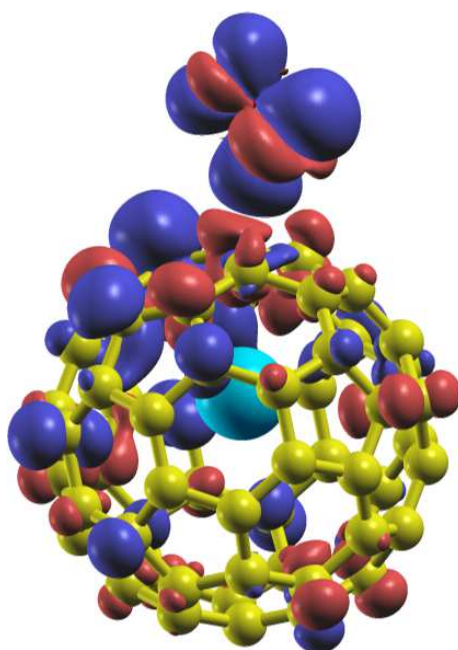
<sup>b</sup> Australian Institute for Nanoscale Science and Technology, and School of Aerospace, Mechanical and Mechatronic Engineering, The University of Sydney, New South Wales, 2006, Australia.



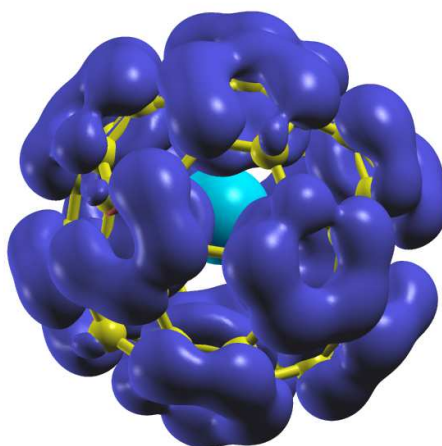
**Fig. 1** (Color online) The spin-density distributions for the Ca@C<sub>60</sub>+NO. The isovalue is  $\pm 0.0005e/\text{\AA}^3$ .



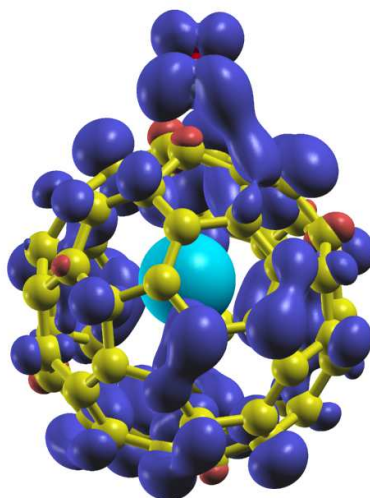
**Fig. 2** (Color online) The spin-density distributions for the Ca@C<sub>60</sub>+NO<sub>2</sub>. The isovalue is  $\pm 0.0005e/\text{\AA}^3$ .



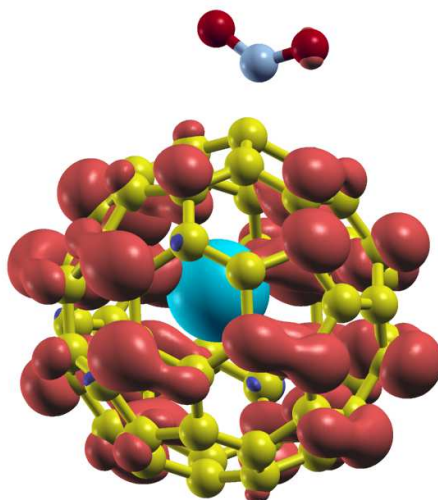
**Fig. 3** (Color online) The spin-density distributions for the Na@C<sub>60</sub>+NO. The isovalue is  $\pm 0.0005 e/\text{\AA}^3$ .



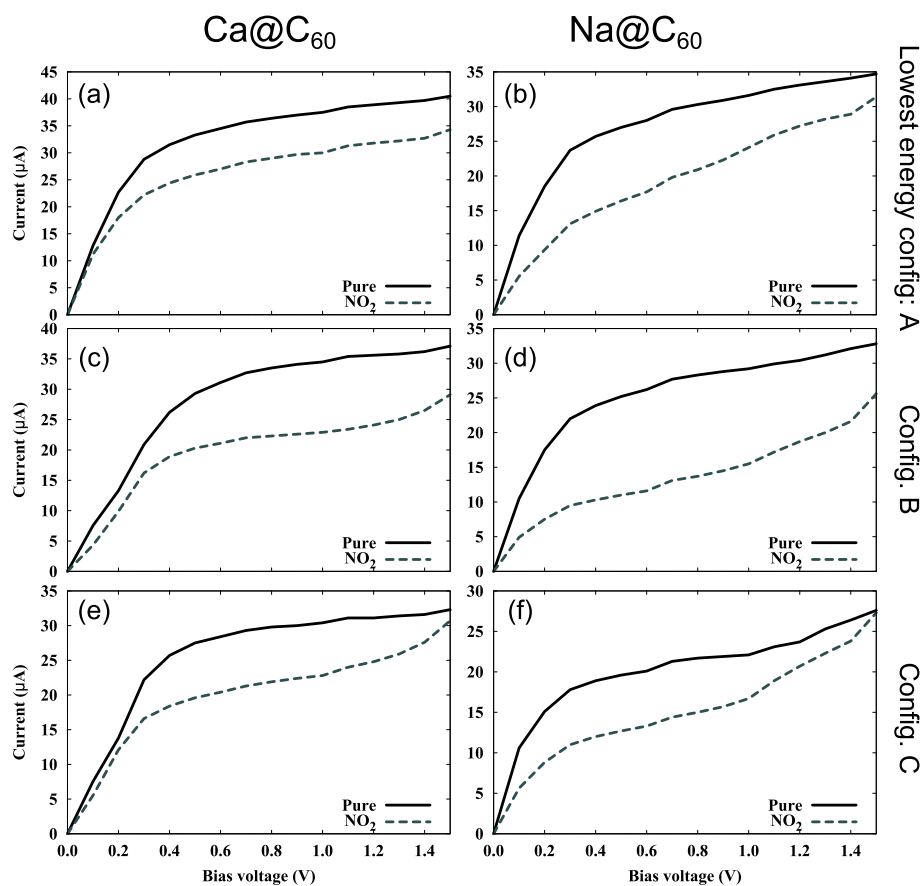
**Fig. 4** (Color online) The spin-density distributions for the Sr@C<sub>60</sub>. The isovalue is  $\pm 0.0005 e/\text{\AA}^3$ .



**Fig. 5** (Color online) The spin-density distributions for the Sr@C<sub>60</sub>+NO. The isovalue is  $\pm 0.0005e/\text{\AA}^3$ .



**Fig. 6** (Color online) The spin-density distributions for the Sr@C<sub>60</sub>+NO<sub>2</sub>. The isovalue is  $\pm 0.0005e/\text{\AA}^3$ .



**Fig. 7** (Color online) The current-voltage characteristics (IVC) for the Na@C<sub>60</sub> and Ca@C<sub>60</sub> systems for pure (without NO<sub>2</sub> adsorption) and with NO<sub>2</sub> adsorption. The lowest energy configurations (as shown in Fig. 4 in the manuscript) are repeated here in parts (a) and (b). The IVC for the two alternative configurations B and C (described in the main text) are shown in parts (c-f).