

## Supplementary Material

### Fullerenes containing water molecules: a study of reactive molecular dynamics simulations

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Additional information, including velocities of the centers of mass for the  $C_{60}$ ,  $H_2O@C_{60}$ , and  $(H_2O)_2@C_{60}$  in the directions of x, y, and z with (a) negative and positive signs, and (b) positive signs and video of the direction of the dipole moment and the orientation of hydrogen and oxygen atoms in the  $H_2O@C_{60}$  (video number one) complex.

**Figure SM1. Velocities of the centers of mass for the  $C_{60}$ ,  $H_2O@C_{60}$ , and  $(H_2O)_2@C_{60}$  in the directions of x (blue), y (red), and z (green) with (a) negative and positive signs, and (b) positive signs.**

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Figure SM1a

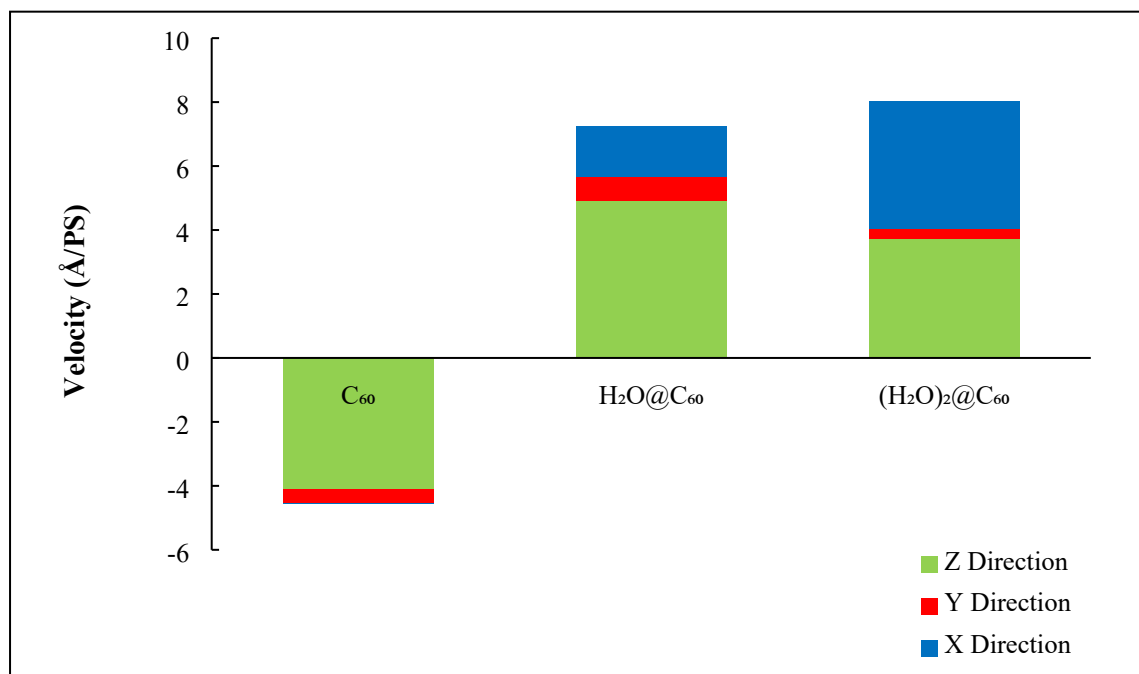
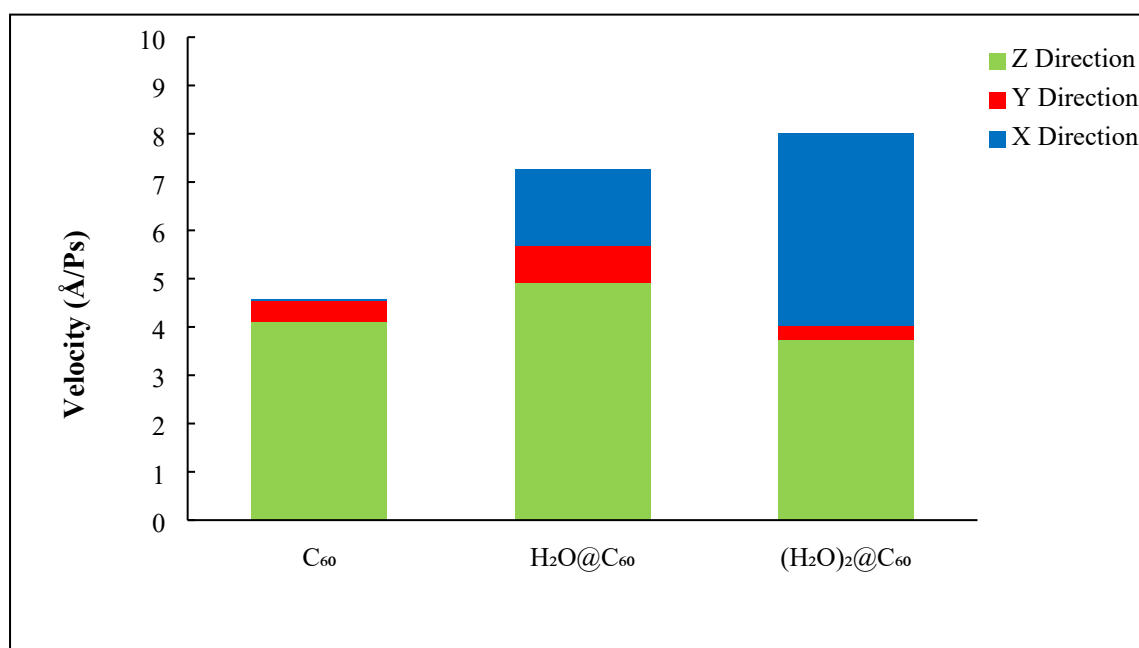


Figure SM1b



**Figure SM2. Video of the direction of the dipole moment in H<sub>2</sub>O@C<sub>60</sub> complex.**

This video was sent to the journal as supporting information-video

