7 Supporting Information

Momentum distributions for the remaining \(2a_2 + 4b_1, 4b_2, 3b_1 + 5a_1, 2b_1 + 4a_1, 1a_2 + 3a_1, 2a_1 + 1b_1\) and \(1b_2\) orbitals of NBD are respectively presented in Figures 8-14. The legends are as follows:

**Figure 8:** The 1500 eV symmetric noncoplanar MD for the \(2a_2 + 4b_1\) orbitals \((\epsilon_f = 11.4 \text{ eV})\). The legend is the same as that for Figure 3.

**Figure 9:** The 1500 eV symmetric noncoplanar MD for the \(4b_2\) orbital \((\epsilon_f = 12.2 \text{ eV})\). The legend is the same as that for Figure 3.

**Figure 10:** The 1500 eV symmetric noncoplanar MD for the \(3b_1 + 5a_1\) orbitals. The legend is the same as that for Figure 3.

**Figure 11:** The 1500 eV symmetric noncoplanar MD for the \(2b_1 + 4a_1\) orbitals. The legend is the same as that for Figure 3 except \((- - - -)\) represents \(0.80 \times (2b_1 + 4a_1)\) MD for BP/TZVP.

**Figure 12:** The 1500 eV symmetric noncoplanar MD for the \(1a_2 + 3a_1\) orbitals. The legend is the same as that for Figure 3 except \((- - - -)\) represents \(0.70 \times (1a_2 + 3a_1)\) MD for BP/TZVP.

**Figure 13:** The 1500 eV symmetric noncoplanar MD for the \(2a_1 + 1b_1\) orbitals. The legend is the same as that for Figure 3 except \((- - - -)\) represents \(0.55 \times (2a_1 + 1b_1)\) MD for BP/TZVP.

**Figure 14:** The 1500 eV symmetric noncoplanar MD for the \(1b_2\) orbital. The legend is the same as that for Figure 3 except \((- - - -)\) represents \(0.55 \times 1b_2\) for BP/TZVP.
Figure 8
Figure 10
Figure 12
Figure 13
Figure 14