Uploaded the attached four xyz files as Supplementary Materials.

Followings are the brief explanations for these files:

MD_Mo_previous.xyz ... MD trajectory of Mo insertion with 40 eV (Fig.3: 0-191 fs) visualizable with VMD.

MD_Mo_continue.xyz ... MD trajectory of Mo insertion with 40 eV (continued: 192-581 fs) visualizable with VMD.
Due to the periodic boundary condition of the simulation cell box, a part of C60 penetrates the cell boundary and appears from the opposite boundary.

MD_Au_previous.xyz ... MD trajectory of Au insertion with 80 eV (Fig.5: 0-249 fs) visualizable with VMD.

MD_Au_continue.xyz ... MD trajectory of Au insertion with 80 eV (continued: 250-767 fs) visualizable with VMD.
Due to the periodic boundary condition of the simulation cell box, a part of C60 penetrates the cell boundary and appears from the opposite boundary.