

Electronic supplementary information for

Locally Spontaneous Dynamic Oxygen Migration on Biphenylene: A DFT Study

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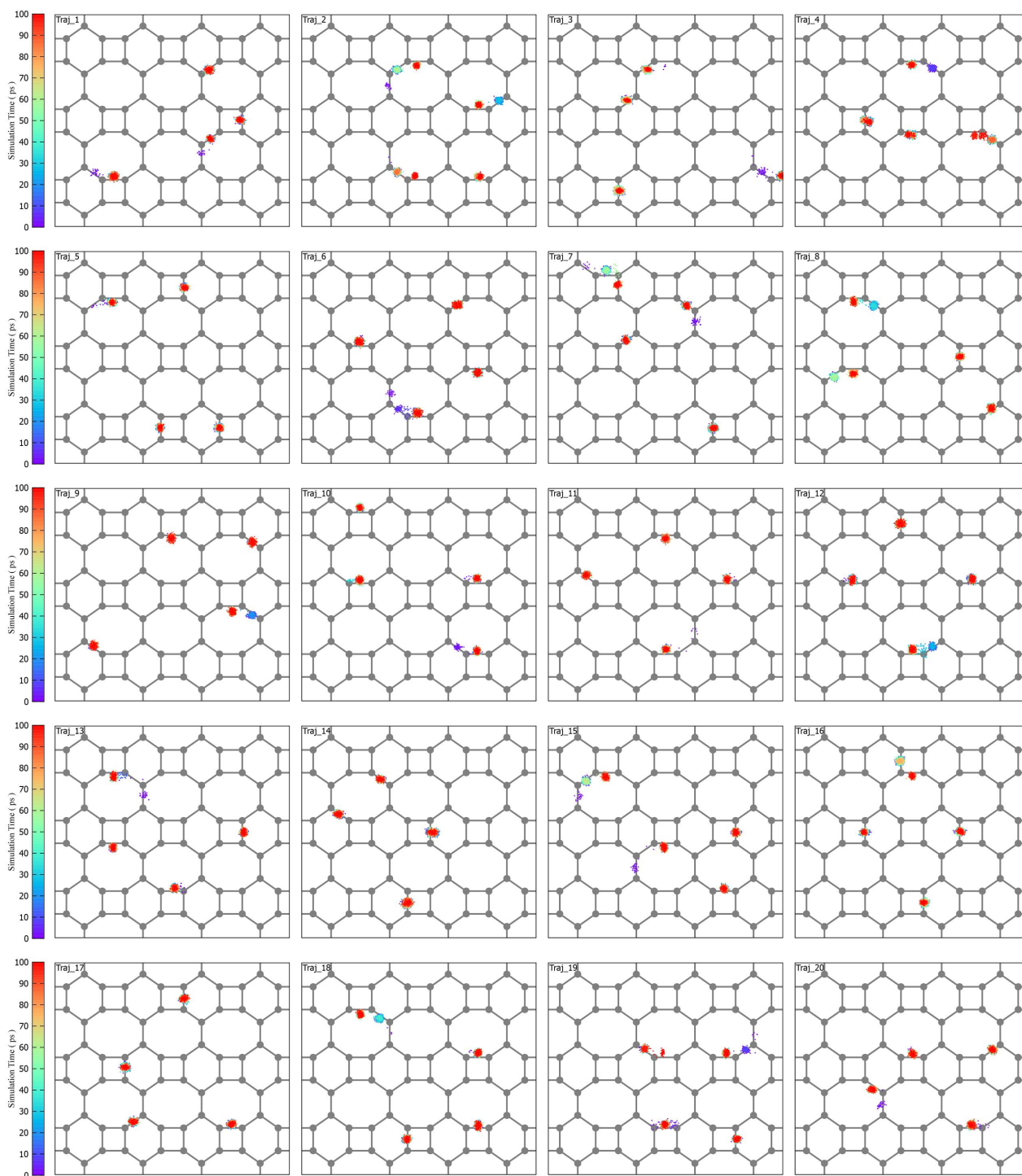
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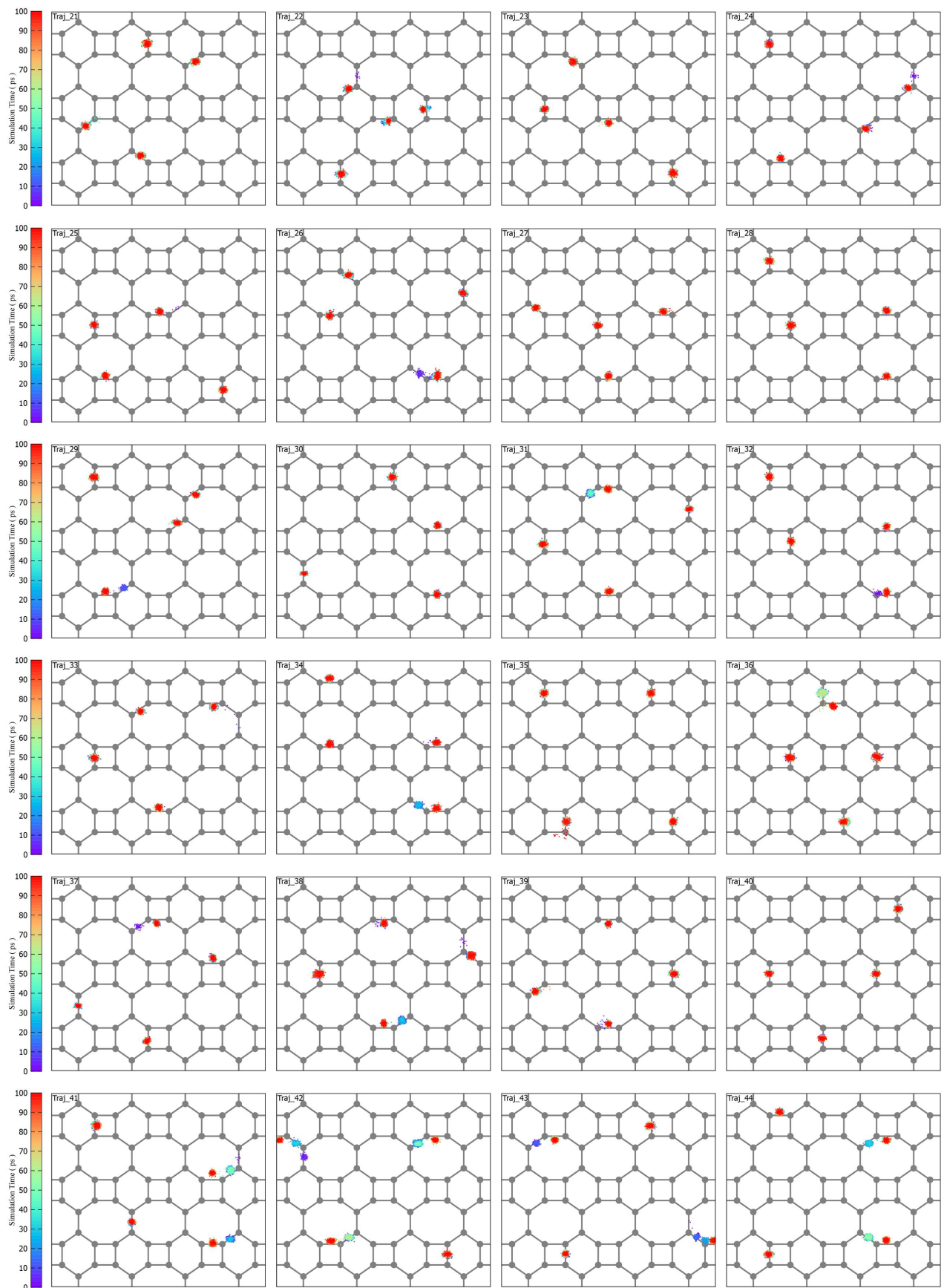
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PS. 1. Sixty trajectories of oxygen atoms on biphenylene monolayer starting from different initial configurations

To clearly show the oxygen migrations in 60 trajectories starting from different initial configurations with 4 randomly distributed epoxy groups, we plotted color-mapped scatter figures. As listed in Fig. S1, the positions of 4 oxygen atoms were extracted and plotted as scatters of 0.05 ps interval for each trajectory, and the simulation time was mapped to different colors. The Traj_16, Traj_44 and Traj_7 were used as the representative illustrations of oxygen migration in Fig. 5 in the manuscript.





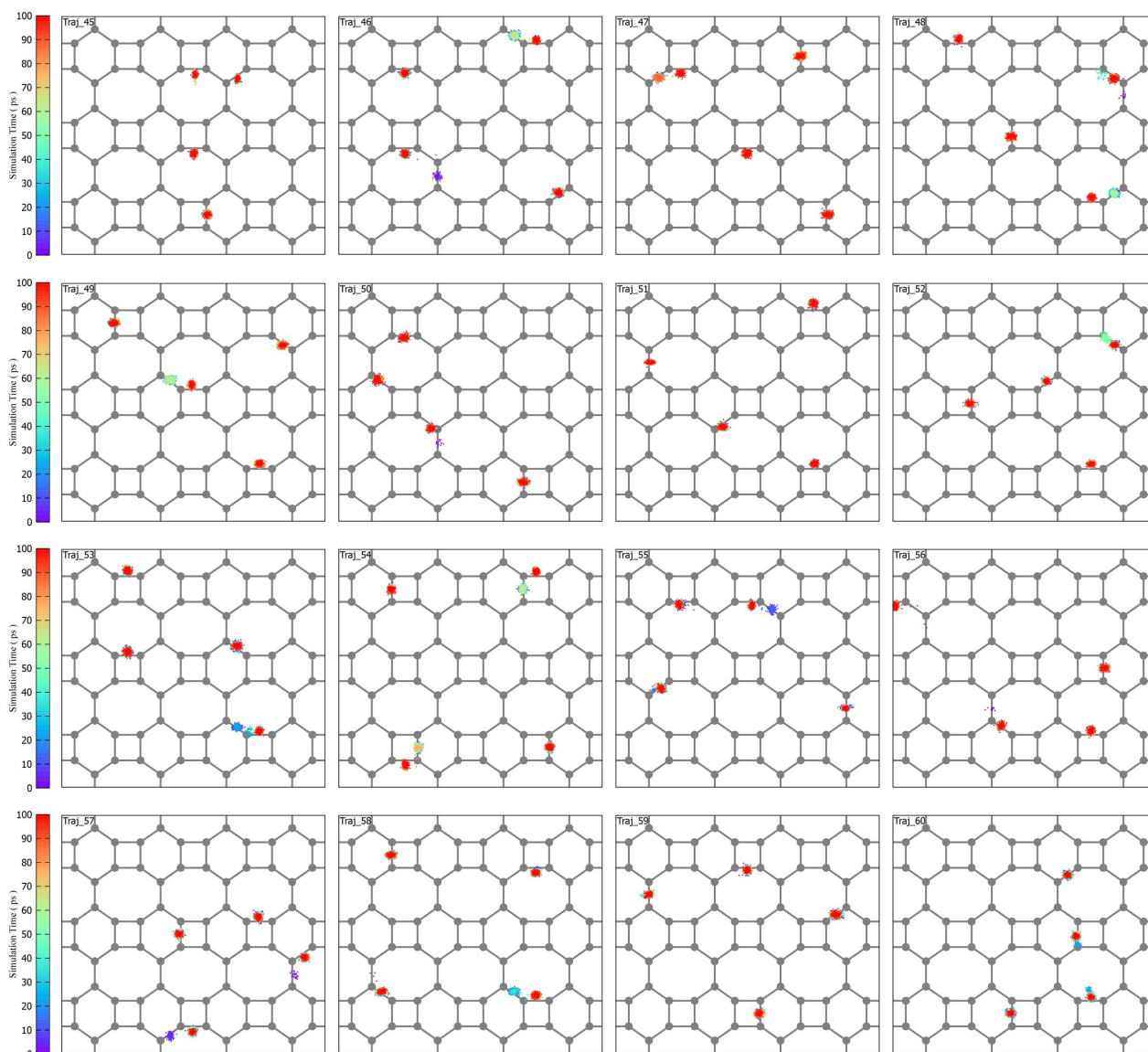


Fig. S1 Sixty MLMD trajectories of oxygen migration on the biphenylene monolayer using the SVD-based MLFF MLMD simulations. The colored dots denote the positions of 4 oxygen atoms, and the colors denote the simulation time. The label in the upper left denotes the index of trajectory. The static biphenylene monolayer is used as the background for clarity. The surface fluctuation of the biphenylene monolayer during the MLMD simulations is not shown therefore the position of epoxy may slightly deviate from the center of C-C bond.

PS. 2. Oxygen migration rate along different reaction pathways

Table S1. Calculated oxygen migration rate of different reaction pathways. Notations: attempt frequency (ν), an elementary length for migration (d), energy barrier (ϵ), and oxygen migration rate (D).

Reaction pathways	ν (THz)	d (Å)	ϵ (eV)	D (cm ² /s)
$B_{8-8} \rightarrow B_{6-8}$	16.62	1.20	0.13	1.58×10^{-5}
$B_{6-8} \rightarrow B_{8-8}$	19.33	1.20	1.49	2.88×10^{-28}
$B_{6-8} \rightarrow B_{6-8}$	17.75	1.20	0.81	6.71×10^{-17}
$B_{6-8} \rightarrow T$	15.87	0.78	0.19	6.36×10^{-7}
$T \rightarrow B_{6-8}$	4.42	0.78	0.14	1.22×10^{-6}
$T \rightarrow B_{4-8}$	8.44	0.61	0.03	9.80×10^{-5}
$B_{4-8} \rightarrow T$	27.83	0.61	0.26	4.50×10^{-8}
$T \rightarrow B_{4-6}$	4.18	1.03	0.19	2.87×10^{-7}
$B_{4-6} \rightarrow T$	13.54	1.03	0.28	2.88×10^{-8}