

# P5620: ADIABATIC MOLECULAR ORBITAL TRACKING IN *AB INITIO* MOLECULAR DYNAMICS FOR 2021 VIRTUAL ISMS

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- New tool to visualize/track real-time electronic structure information in AIMD trajectories.
- Temporal orbital character mapping between AIMD steps.

$$M_{ij} \approx \begin{matrix} & |\phi_i\rangle & |\phi_j\rangle \\ \begin{matrix} \langle\phi_i| \\ \langle\phi_j| \end{matrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{matrix} \text{MO Phase Switch} \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{matrix} & \begin{matrix} \text{MO Order Switch} \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{matrix}$$

