Electronic Supplementary Information

Using Ab Initio Molecular Dynamics to Examine Competitive O₂/N₂ Adsorption at Open Metal Sites of M₂(dobdc)

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Figure ESI-2. Average M-N$_2$ bond distances for single-component N$_2$ systems, for (a) bent and (b) linear N$_2$ molecules. Bent molecules were those with an M-N-N angle between 80° and 165°; linear molecules had M-N-N angles between 165° and 180°.
**Figure ESI-3.** Average M-O-O angles for single-component O₂ systems, for (a) side-on and (b) bent O₂ molecules. Side-on bound molecules were those with an M-O-O angle between 67° and 80°; bent molecules had M-O-O angles between 80° and 165°.
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