Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Using *Ab Initio* Molecular Dynamics to Examine Competitive O_2/N_2 Adsorption at Open Metal Sites of M_2(dobdc)

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Contents

Figure ESI-1 Average M-O_2 bond distances 2
Figure ESI-2 Average M-N_2 bond distances 3
Figure ESI-3 Average M-O-O angles 4
Figure ESI-4 Average M-N-N angles 5
Figure ESI-5 Time evolution of adsorption for Fe_2(dobdc)/4:6 O_2:N_2 6

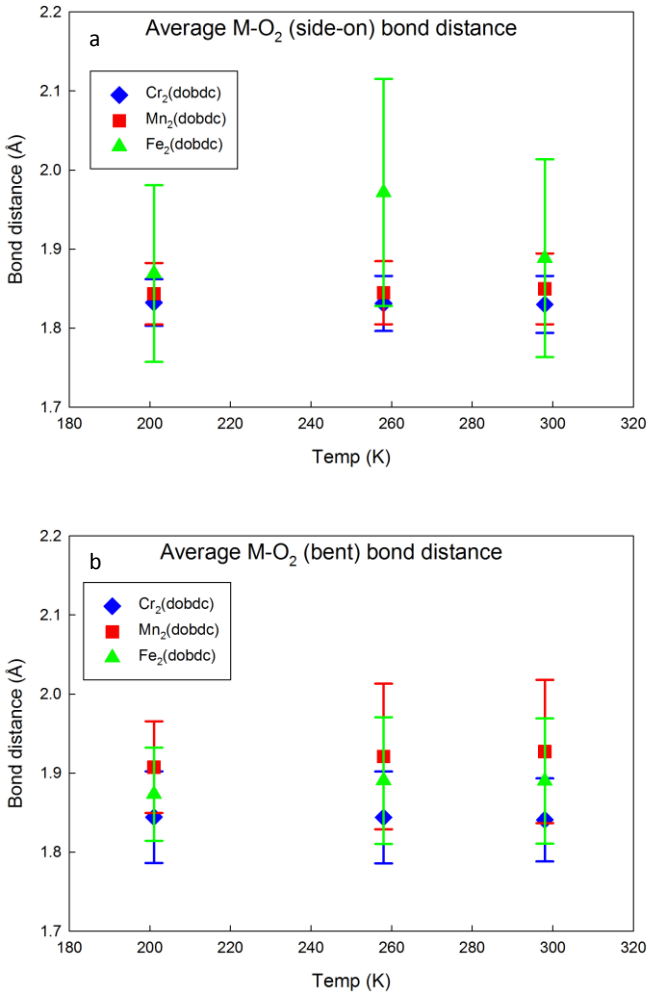

Figure ESI-1. Average M-O_2 bond distances for single-component O_2 systems, for (a) side-on bound and (b) bent O_2 molecules. Side-on bound molecules were those with an M-O-O angle between 67° and 80°; bent molecules had M-O-O angles between 80° and 165°.

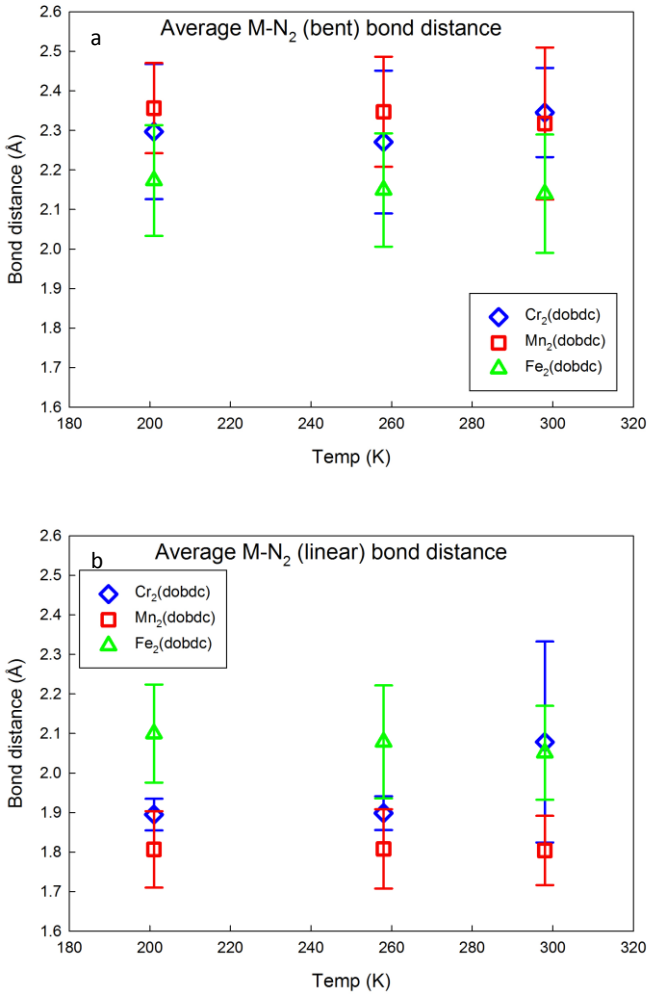

Figure ESI-2. Average M-N_2 bond distances for single-component N_2 systems, for (a) bent and (b) linear N_2 molecules. Bent molecules were those with an M-N-N angle between 80° and 165°; linear molecules had M-N-N angles between 165° and 180°.

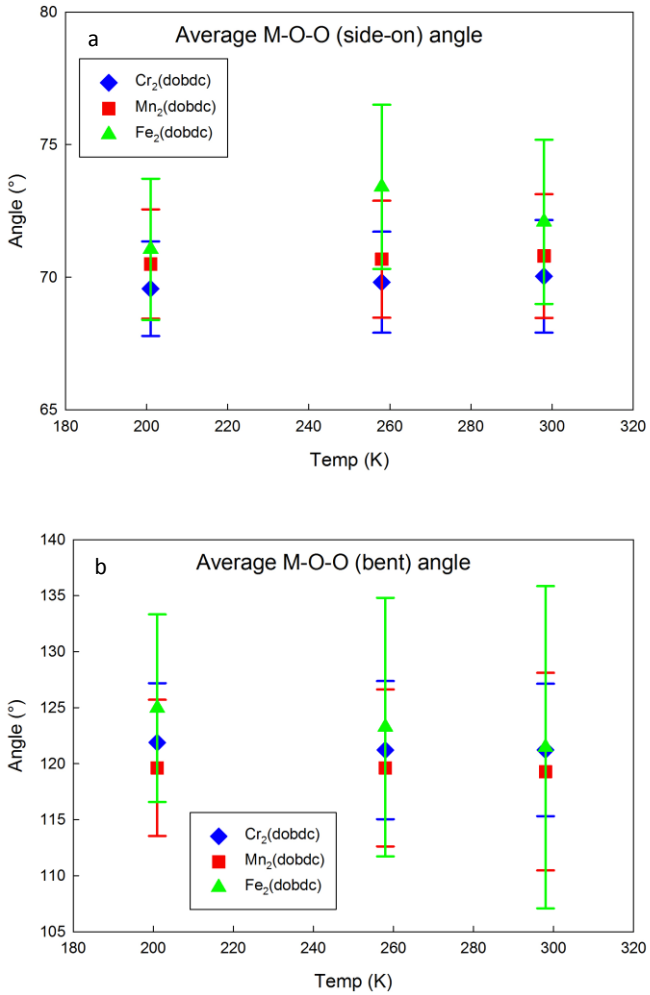

Figure ESI-3. Average M-O-O angles for single-component O_2 systems, for (a) side-on and (b) bent O_2 molecules. Side-on bound molecules were those with an M-O-O angle between 67° and 80°; bent molecules had M-O-O angles between 80° and 165°.

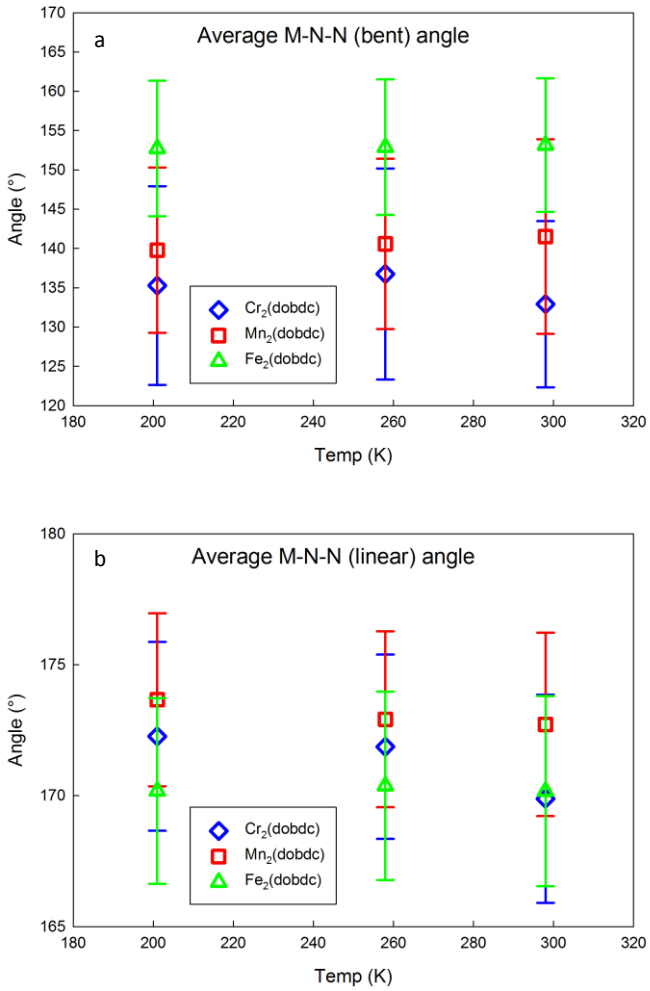

Figure ESI-4. Average M-N-N angles for single-component N_2 systems, for (a) bent and (b) linear N_2 molecules. Bent molecules were those with an M-N-N angle between 80° and 165°; linear molecules had M-N-N angles between 165° and 180°.

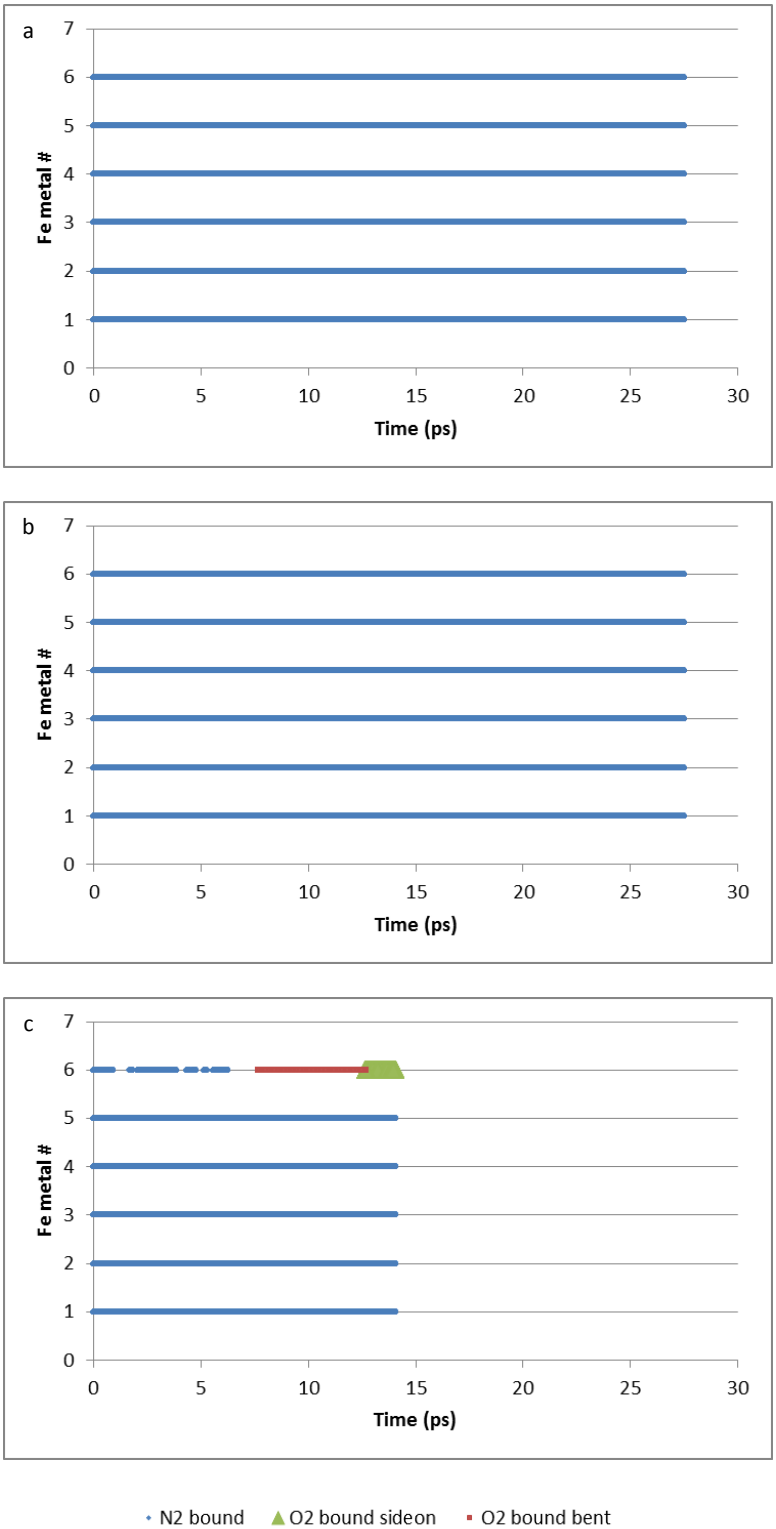

Figure ESI-5. Plots of N_2 and O_2 bound to each Fe metal center of Fe_2(dobdc) over time, for 4:6 O_2:N_2 loadings, at (a) 201 K, (b) 258 K, and (c) 298 K. Each simulation begins with six molecules of N_2 bound to the six metal centers and four molecules of O_2 in the center of the pore.