Electronic Supplementary Material (ESI) for RSC Advances.

Band gap of noble and transition metal /ZIF-8 electro/catalysts: A computational study

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Figure S1 to **Figure S8** indicate the band structures and projected density of states by addition of Ni, Mn, Co, Pd, Pt, Cu, Fe, and Ti atoms to pristine ZIF-8 framework. As can be seen, the bandgap values were decreased significantly by addition of Fe and Ti to this structure.

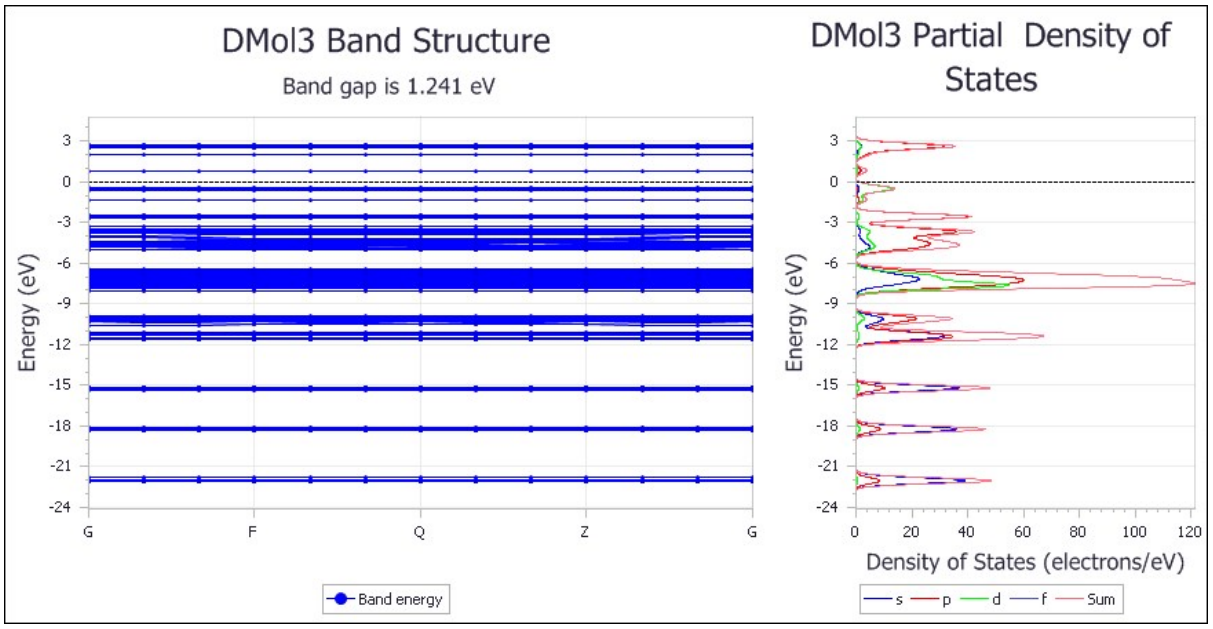

Figure S1: band structure and projected density of states for Co/ZIF-8

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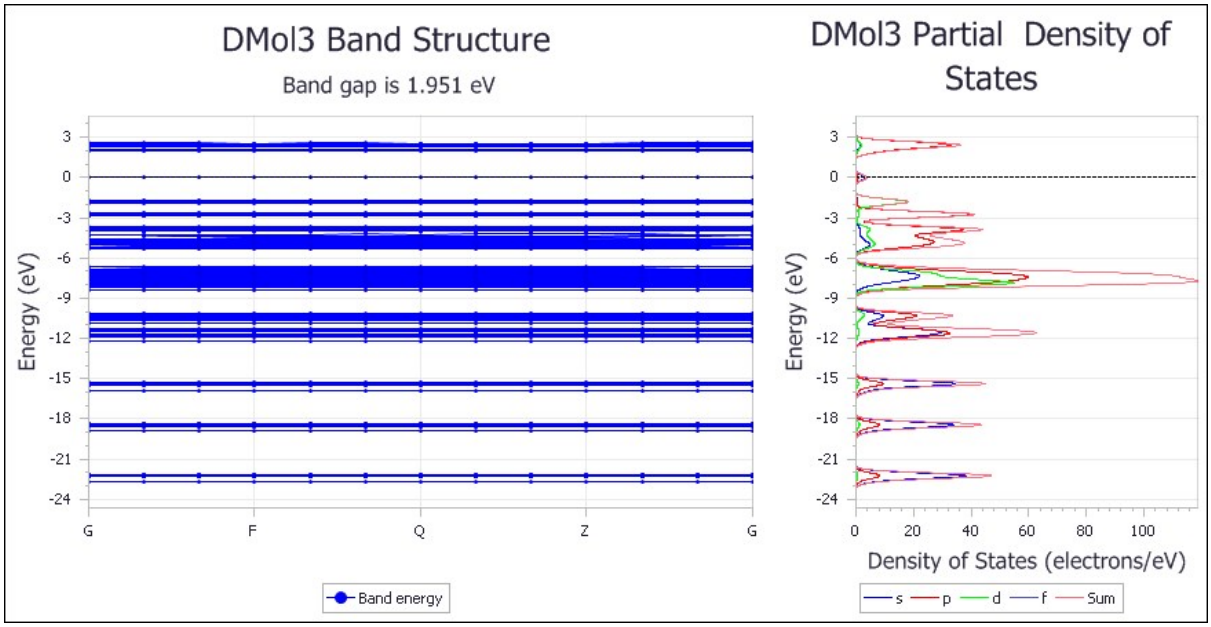

Figure S2: band structure and projected density of states for Cu/ZIF-8

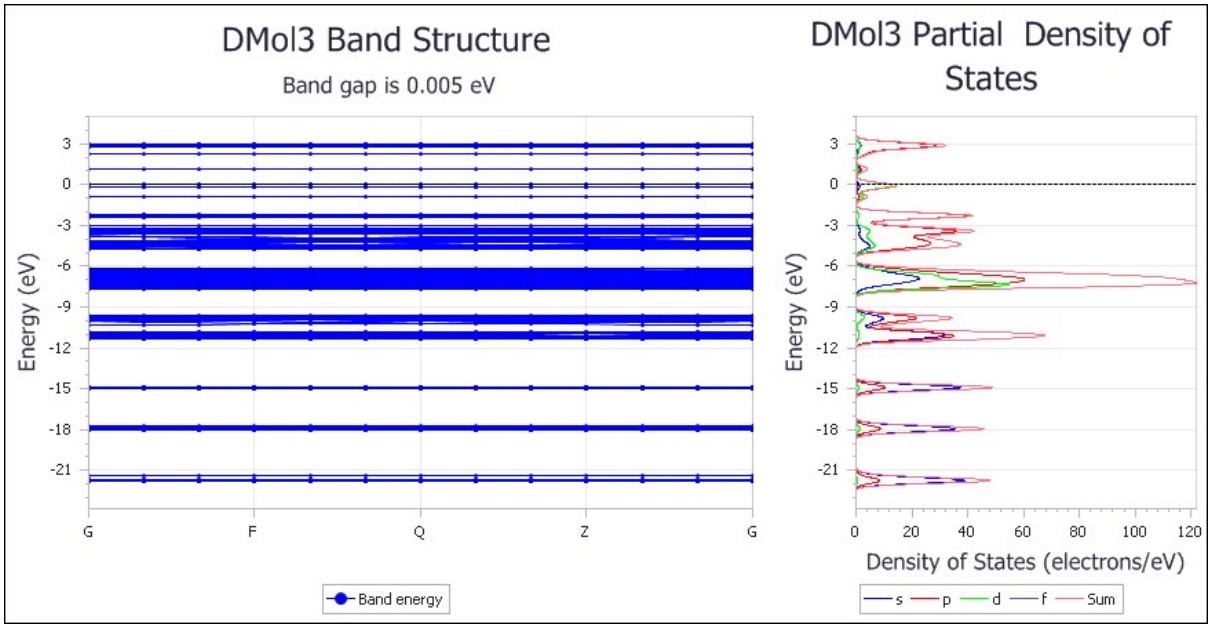

Figure S3: band structure and projected density of states for Fe/ZIF-8

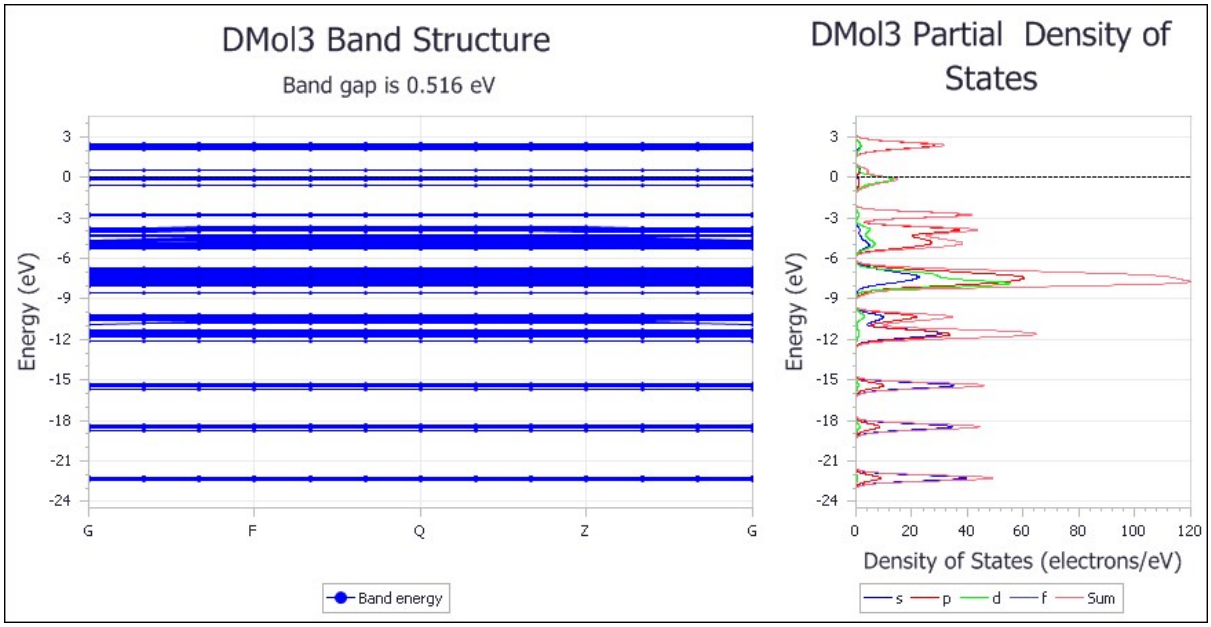

Figure S4: band structure and projected density of states for Mn/ZIF-8

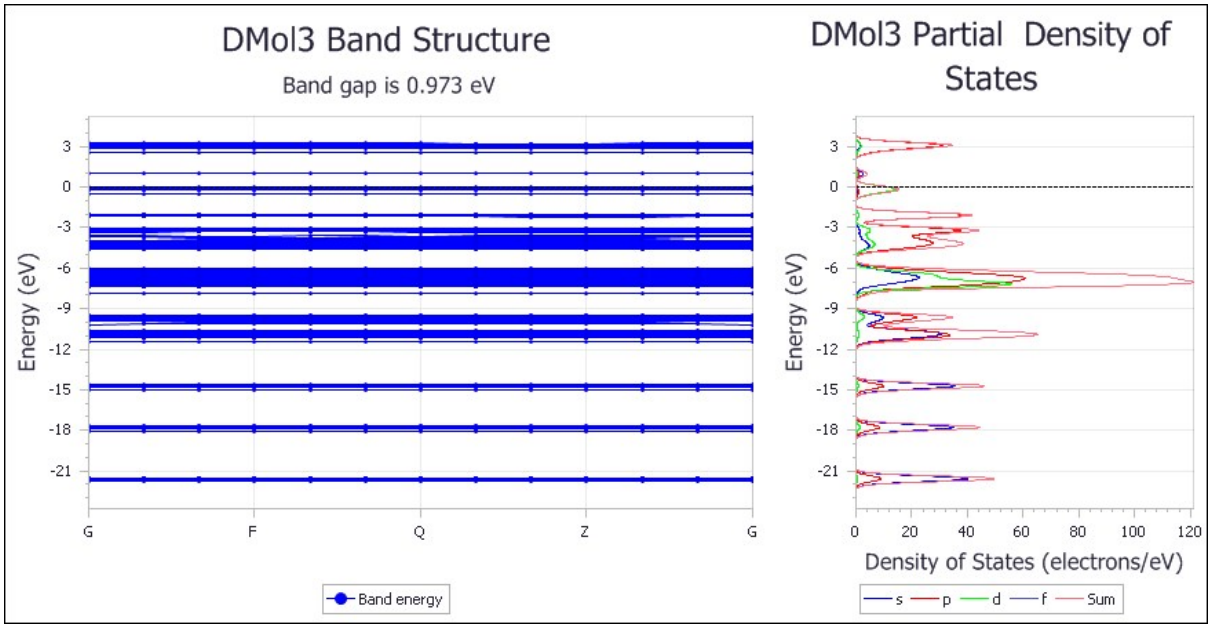

Figure S5: band structure and projected density of states for Ni/ZIF-8

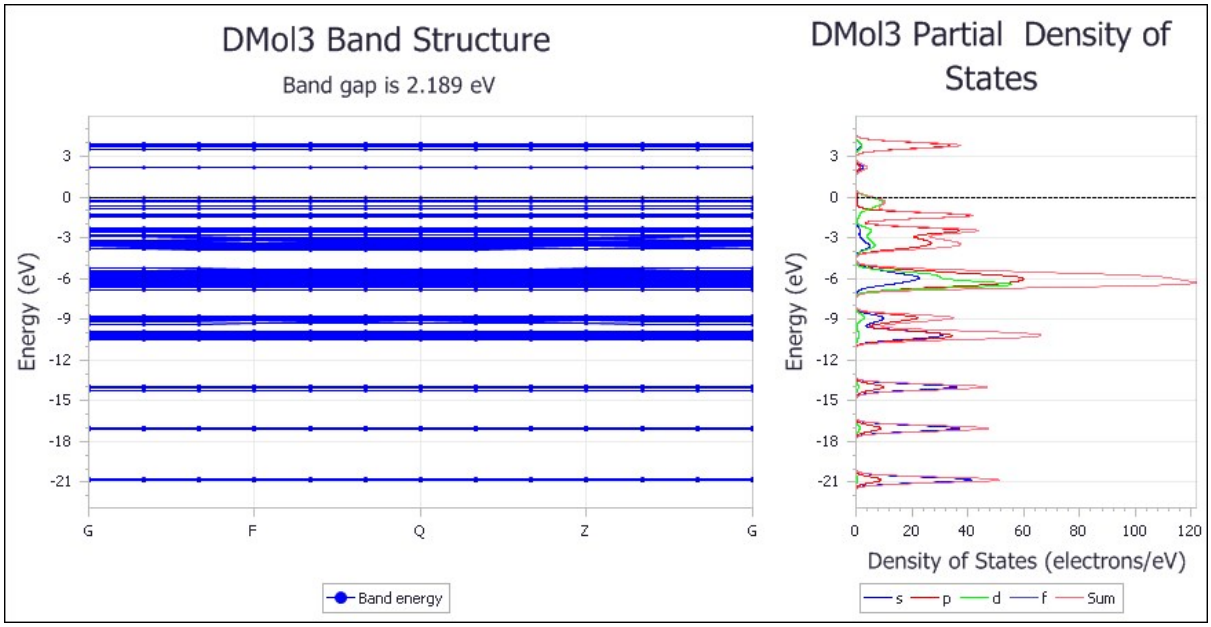

Figure S6: band structure and projected density of states for Pd/ZIF-8

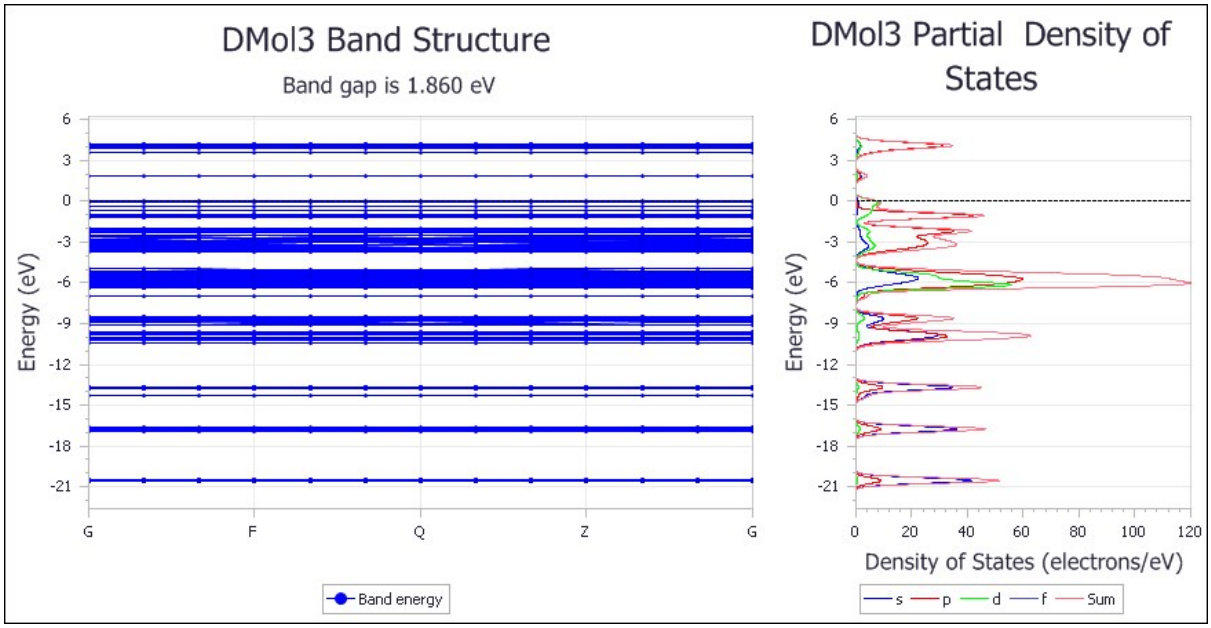

Figure S7: band structure and projected density of states for Pt/ZIF-8

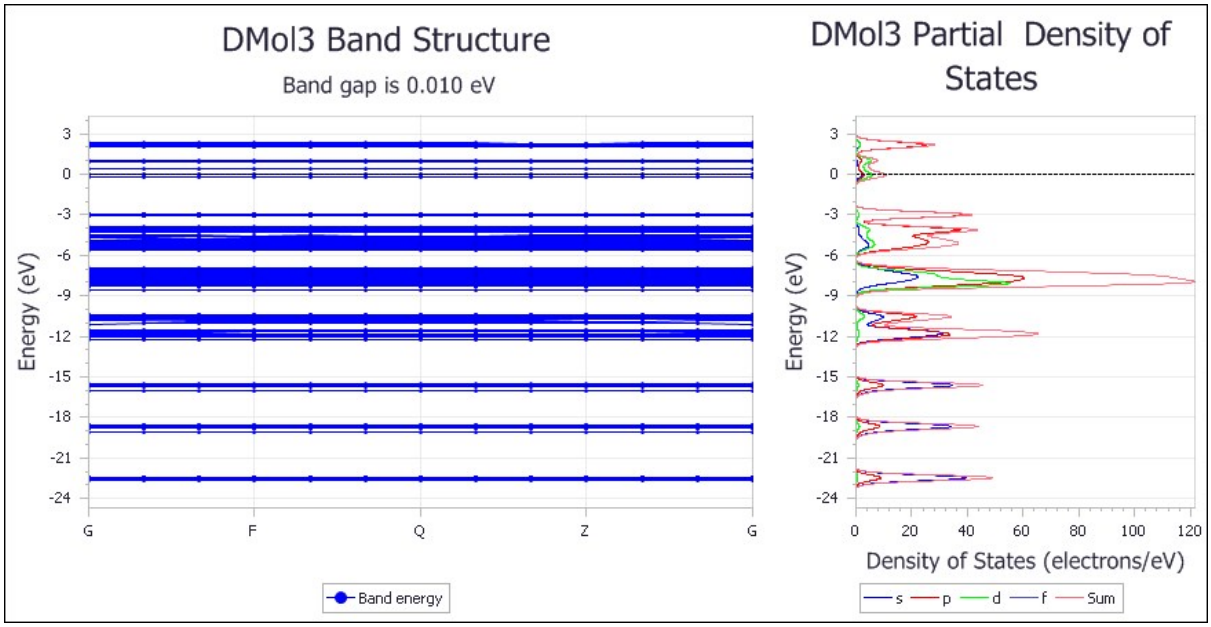

Figure S8: band structure and projected density of states for Pt/ZIF-8