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Computational design of metal-organic frameworks with paddlewheel-type secondary building units UDO SCHWINGENSCHLOGL, MAXIM V. PESKOV, NEJIB MASGHOUNI, PSE Division, KAUST, Thuwal 23955, Saudi Arabia — We employ the TOPOS package to study 697 coordination polymers containing paddlewheel-type secondary building units. The underlying nets are analyzed and 3 novel nets are chosen as potential topologies for paddlewheel-type metal organic frameworks (MOFs). Dicarboxylate linkers are used to build basic structures for novel isoreticular MOF series, aiming at relatively compact structures with a low number of atoms per unit cell. The structures are optimized using density functional theory. Afterwards the Grand Canonical Monte Carlo approach is employed to generate adsorption isotherms for CO_2, CO, and CH_4 molecules. We utilize the universal forcefield for simulating the interaction between the molecules and hosting MOF. The diffusion behavior of the molecules inside the MOFs is analyzed by molecular dynamics simulations.

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