

# Addressing challenges of identifying geometrically diverse sets of crystalline porous materials

Richard Luis Martin,<sup>a</sup> Berend Smit,<sup>b,c</sup> Maciej Haranczyk<sup>a</sup>

<sup>a</sup> *Computational Research Division, Lawrence Berkeley National Laboratory, One Cyclotron Road, Mail Stop 50F-1650, Berkeley, CA 94720-8139*

<sup>b</sup> *Department of Chemistry, University of California, Berkeley, CA 94720-1462*

<sup>c</sup> *Department of Chemical Engineering, University of California, Berkeley, CA 94720-1462*

## SUPPLEMENTARY INFORMATION

Framework IDs for the 174 diverse hypothetical zeolites, in the order of selection (beginning with the seed, 8000013):

8000013	8328249	8092879	8210209	8266780	8314968
8114390	8319868	8315341	8315642	8328987	8292068
8091197	8326549	8272636	8266752	8292734	8312661
8208290	8306514	8067994	8203028	8116163	8199595
8210505	8082973	8209475	8195254	8288137	8307680
8299445	8196911	8255526	8320264	8265147	8197407
8297518	8330551	8274758	8206292	8321333	8208795
8274251	8304004	8196860	8317776	8091453	8330405
8193503	8194213	8325802	8315933	8319370	8218318
8293981	8243805	8274185	8193579	8255452	8306594
8059336	8265888	8328395	8328286	8052774	8314692
8200248	8312646	8330409	8310018	8206921	8319591
8238982	8287150	8319642	8206467	8316737	8323306
8306803	8193801	8093500	8317391	8064074	8328879
8307351	8185843	8315792	8291835	8266562	8092670
8063072	8167979	8202869	8312222	8196431	8271394
8193613	8240531	8117135	8200972	8268229	8307072
8311043	8291039	8321618	8064650	8316162	8196375
8208070	8270799	8293801	8178205	8288480	8244206
8267222	8265164	8207615	8313981	8271340	8286995
8177958	8067517	8329208	8316395	8314022	8299597
8325094	8297616	8284797	8323077	8286170	8326862
8205074	8330766	8323246	8288642	8309270	8323161
8080292	8196092	8323420	8319944	8297934	8289385
8311152	8316949	8321868	8081567	8291930	8212201
8313764	8195101	8197781	8261549	8268915	8274897
8280064	8312713	8316608	8299453	8196815	8330092
8288136	8319686	8319489	8315874	8271239	8315086

8292776

8288477

8329249

8323321

8267574

8098063