

README: list of the archives found as supplementary information.

1.- Root directory:

1a.- This README file

1b.- Ordered_Nanoporous_Metals_Supp_Information.docx: The file has 14 sections and two additional sections for describing metadynamics codes.

List of sections:

Section S1. EAM Potentials

Section S2. Lattice energy and cell parameter time dependence for Pt-CRI-ST3

Section S3. NVT stability of Ni-CRI-ST3 ONM

Section S4. Metadynamics simulations

Code S1: Plumed code used in the MetaD simulation

Code S2: Reweighting and calculating the histograms

Section S5.- Calculation of the thermal expansion coefficient, α , and the specific heat, C_p .

Section S6.- Calculation of mean-squared displacements of methanol and water Ag-CRI ST3 ONM

Section S7.- List of stable ONMs structures designed in this work

Section S8.- Views of stable ONMs structures

Section S9.- Energy per atom vs density for Ni and Pt ONMs with alternative potentials

Section S10.- Porosities of stable ONMs

Section S11.- Empirical formula for calculating the critical PLD of stable ONMs

Section S12.- Porosities and stabilities of template MOFs and ST solids

Section S13.- Distribution of adsorption enthalpies and transport of benzene and xylene isomers

Section S14.- References

2.- ONMs_Crystal_Structures directory

Cif files of our predicted ONMs:

2.1. ONM_from_MOF_IRMOF16.cif

2.2. ONM_from_MOF_NDC-MIL101.cif

2.3. ONM_from_MOF_PCN6P.cif

2.4. ONM_from_ST_CRI-ST3.cif

2.5. ONM_from_ST_CRI-ST4.cif

2.6. ONM_from_ST_SOD-ST3.cif

2.7. ONM_from_ST_SOD-ST4.cif

3.- ONMs_EAM_Potential_files directory

EAM files:

3.1. EAM_Ag.Sheng.lammps.eam

3.2. EAM_Au.Sheng.lammps.eam

3.3. EAM_Ni.OrtizRoldan.eam

3.4. EAM_Ni.Sheng.lammps.eam

3.5. EAM_Pd.Sheng.lammps.eam

3.6. EAM_Pt.Johnson.lammps.eam

3.7. EAM_Pt.Sheng.lammps.eam

4.- Xylenes_Ag_CRIST3_Diffusion directory

RASPA files to run MD simulations of ortho, meta and paraxylene in Ag_CRISTobalite ONM:

4.1. 1a_ag_CRIST3_ortho_xylene_jalkanen

4.2. 1b_ag_CRIST3_meta_xylene_jalkanen

4.3. 1c_ag_CRIST3_para_xylene_jalkanen