# Supporting Materials for: Molecular Methods for Assessing the Morphology, Topology, and Performance of Polyamide Membranes

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## S1. Molecular Dynamics Force Field Parameters and Atomic Partial Charges

We utilized the General Amber Force Field (GAFF) to define bonded interaction parameters including those for bonds, angles, dihedrals, and impropers. Figure S1 shows the locations of the atoms defined by their symbols, with subscript numbers indicating variations of otherwise identical atoms that only differ based upon charge. GAFF was also used to define Lennard Jones $\sigma$ and $\varepsilon$ values. The AM1-BCC method was used to assign atomic partial charges to the monomers, MPD-TMC oligomer, hydroxide, and hexane. The TIP3P water model was used to define bond, angle, partial charge, and Lennard Jones parameters for water molecules. Table S1 contains all atom-specific force field information, including mass, Lennard Jones parameters, and atomic partial charge. Tables S2-S5 contains all bond, angle, improper, and dihedral force field constants, respectively.

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Table S1: Mass $m$, Lennard Jones parameters $\varepsilon$, $\sigma$, and partial charge $q$ for each atom type used in simulations of polyamide polymerization, hydration, equilibration, and operation.

| Name | Symbol | $m$ (Da) | $\varepsilon$ (Kcal.mol$^{-1}$) | $\sigma$ (Å) | $q$ (e) |
|---|---|---|---|---|---|
| Aromatic Carbon | ArC1 | 12.010 | 0.08600 | 3.3996700 | 0.171600 |
| | ArC2 | 12.010 | 0.08600 | 3.3996700 | -0.230000 |
| | ArC3 | 12.010 | 0.08600 | 3.3996700 | -0.156500 |
| | ArC4 | 12.010 | 0.08600 | 3.3996700 | -0.195600 |
| | ArC5 | 12.010 | 0.08600 | 3.3996700 | 0.014000 |
| Aromatic Hydrogen | ArH1 | 1.008 | 0.01500 | 2.5996000 | 0.107450 |
| | ArH2 | 1.008 | 0.01500 | 2.5996000 | 0.181600 |
| Amine Nitrogen | AN | 14.010 | 0.17000 | 3.2500000 | -0.462100 |
| Amine Hydrogen | AH | 1.008 | 0.01570 | 1.0691000 | 0.231050 |
| Acyl Carbon | AcC | 12.010 | 0.08600 | 3.3996700 | 0.679700 |
| Acyl Oxygen | AcO | 16.000 | 0.21000 | 2.9599000 | -0.576100 |
| Acyl Chloride | AcCl | 35.450 | 0.26500 | 3.4709414 | -0.103600 |
| Amide Nitrogen | LN | 14.010 | 0.17000 | 3.2500000 | -0.398375 |
| Amide Carbon | LC | 12.010 | 0.08600 | 3.3996700 | 0.743425 |
| Hydroxyl Oxygen | HyO | 16.000 | 0.21000 | 2.9599000 | -0.535100 |
| Hydroxyl Hydrogen | HyH | 1.008 | 0.01500 | 2.5996000 | 0.431500 |
| Hexane Carbon | HeC | 12.010 | 0.10940 | 3.3996700 | -0.080400 |
| Hexane Hydrogen | HeH1 | 1.008 | 0.01569 | 2.6495440 | 0.032700 |
| | HeH2 | 1.008 | 0.01569 | 2.6495440 | 0.038700 |
| TIP3P Water Oxygen | WO | 16.000 | 0.15210 | 3.1570000 | -0.830000 |
| TIP3P Water Hydrogen | WH | 1.008 | 0.01500 | 2.0580000 | 0.415000 |
| Graphene Piston Carbon | GC | 12.010 | 0.06844 | 3.4070000 | 0.000000 |

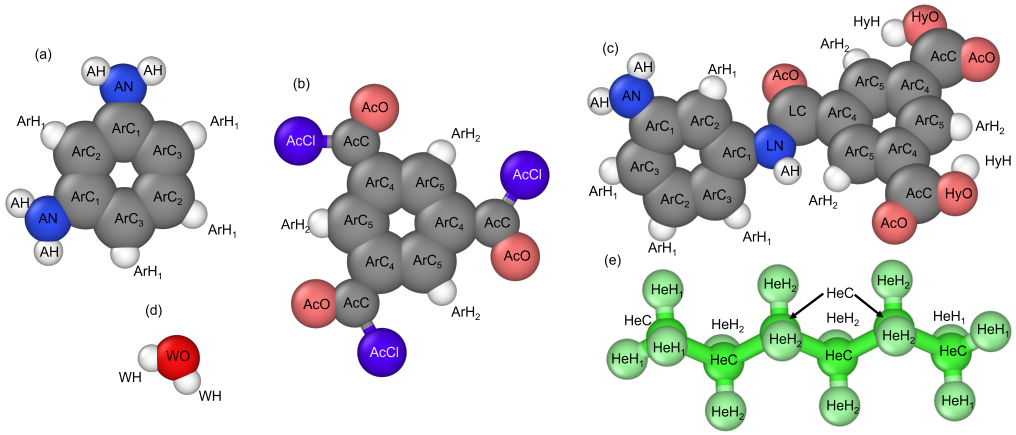


Figure S1: Representative monomers, oligomers, and constituent molecules with corresponding atomic symbols; (a) *m*-phenylenediamine (MPD), (b) trimesoyl chloride (TMC), (c) MPD-TMC oligomer, (d) water, (e) hexane.

## S2. Minkowski Functional Grid Independence Study

Figure S2 shows the Minkowski functionals evaluated for the pore space opening map of a dry 1x domain polymerized domain. Voxel sizes used were 0.4 Å, 0.2 Å, 0.1 Å, and 0.05 Å. The relative error between the finest two resolutions (0.1 Å and 0.05 Å) calculated with an $l^2$-norm was 0.0093, 0.011, 0.057, and 0.032 for the porosity density, surface area density, mean surface curvature density, and Euler characteristic density, respectively. Therefore 0.05 Å is sufficiently small enough to give resolution independent results.

Table S2: Bond force constants $K_b$ and equilibrium bond lengths $r_0$ for all bond types used in simulations of polyamide polymerization, hydration, equilibration, and operation.

| Bonded Atoms | $K_b$ (Kcal.mol$^{-1}$.Å$^{-2}$) | $r_0$ (Å) |
|---|---|---|
| ArC - ArC | 461.1 | 1.3984 |
| ArC - ArH | 345.8 | 1.0860 |
| ArC - AcC/LC | 345.9 | 1.4906 |
| AcC - AcCl | 267.4 | 1.8029 |
| AcO - AcC/LC | 637.7 | 1.2183 |
| AcC - HyO | 400.1 | 1.3513 |
| HyO - HyH | 371.4 | 0.9730 |
| LN - LC | 427.6 | 1.3790 |
| ArC - AN/LN | 417.9 | 1.3859 |
| AH - AN/LN | 404.6 | 1.0121 |
| WO - WH | 450 | 0.9572 |
| HeC - HeC | 300.9 | 1.5375 |
| HeC - HeH | 330.6 | 1.0969 |

Table S3: Bond angle force constants $K_\theta$ and equilibrium bond angles $\theta_0$ for all bond angle types used in simulations of polyamide polymerization, hydration, equilibration, and operation.

| Bonded Atoms | $K_\theta$ (Kcal.mol$^{-1}$) | $\theta_0$ (deg.) |
|---|---|---|
| ArC - ArC - ArC | 66.6 | 120.020052 |
| ArC - ArC - AcC/LC | 64.3 | 120.330052 |
| ArC - ArC - ArH | 48.2 | 119.880051 |
| ArC - AcC/LC - AcO | 68.7 | 122.600053 |
| ArC - AcC - HyO | 69.2 | 113.450049 |
| AcC - HyO - HyH | 49.9 | 106.550046 |
| AcO - AcC - HyO | 75.9 | 122.100052 |
| ArC - ArC - AN/LN | 68.3 | 120.950052 |
| ArC - AN/LN - AH | 48.4 | 116.070050 |
| AH - AN - AH | 40.1 | 115.120050 |
| LC - LN - ArC | 63.8 | 123.710053 |
| LC - LN - AH | 48.3 | 117.550051 |
| LC - LN - ArC | 67.7 | 115.250050 |
| LN - LC - AcO | 74.2 | 123.050053 |
| ArC - AcC - AcCl | 61.1 | 114.705049 |
| AcO - AcC - AcCl | 58.8 | 120.690052 |
| WH - WO - WH | 55 | 104.520000 |
| HeC - HeC - HeC | 62.9 | 111.510048 |
| HeC - HeC - HeH | 46.3 | 109.800047 |
| HeH - HeC - HeH | 39.4 | 107.580046 |

Table S4: Dihedral torsion angle force constants $K_\phi$, periodicity constant $n$, phase shift angle $d$, and weighting factors for all dihedral torsion angle types used in simulations of polyamide polymerization, hydration, equilibration, and operation.

| Bonded Atoms | $K_\phi$ (Kcal.mol$^{-1}$) | $n$ (-) | d (deg.) | Weighting Factor (-) |
|---|---|---|---|---|
| ArC - ArC - ArC - ArC | 3.625 | 2 | 180 | 0.5 |
| ArC - ArC - ArC - ArH | 3.625 | 2 | 180 | 0.0 |
| ArH - ArC - ArC - ArH | 3.625 | 2 | 180 | 0.0 |
| ArH - ArC - ArC - AN/LN | 3.625 | 2 | 180 | 0.0 |
| ArC - ArC - ArC - AN/LN | 3.625 | 2 | 180 | 0.0 |
| ArC - ArC - AN/LN - AH | 0.450 | 2 | 180 | 0.0 |
| ArC - ArC - ArC - AcC/LC | 3.625 | 2 | 180 | 0.0 |
| ArH - ArC - ArC - AcC/LC | 3.625 | 2 | 180 | 0.0 |
| ArC - ArC - AcC/LC - AcO | 1.050 | 2 | 180 | 0.0 |
| ArC - ArC - AcC - AcCl | 1.000 | 2 | 180 | 0.0 |
| ArC - ArC - LN - LC | 0.450 | 2 | 180 | 0.0 |
| ArC - LC - LN - ArC | 2.300 | 2 | 180 | 0.0 |
| ArC - LC - LN - AH | 2.300 | 2 | 180 | 0.0 |
| ArC - ArC - LC - LN | 1.050 | 2 | 180 | 0.0 |
| ArC - LN - LC - AcO | 2.300 | 2 | 180 | 0.0 |
| AH - LN - LC - AcO | 2.300 | 2 | 180 | 0.0 |
| ArC - ArC - AcC/LC - AcO | 1.000 | 2 | 180 | 0.0 |
| ArC - AcC - HyO - HyH | 2.300 | 2 | 180 | 0.0 |
| AcO - AcC - HyO - HyH | 2.300 | 2 | 180 | 0.0 |
| HeC - HeC - HeC - HeC | 0.250 | 2 | 180 | 0.0 |
| HeC - HeC - HeC - HeH | 0.160 | 3 | 0 | 0.0 |
| HeH - HeC - HeC - HeH | 0.150 | 3 | 0 | 0.0 |

Table S5: Improper dihedral angle force constants $K_\chi$ and equilibrium improper dihedral angles $\chi_0$ for all improper dihedral angle types used in simulations of polyamide polymerization, hydration, equilibration, and operation.

| Bonded Atoms | $K_\chi$ (Kcal.mol$^{-1}$) | $\chi_0$ (deg.) |
|---|---|---|
| ArC - ArC - ArC - ArH | 1.1 | 180 |
| ArC - ArC - ArC - AN/LN | 1.1 | 180 |
| ArC - ArC - ArC - AcC/LC | 1.1 | 180 |
| ArC - LC - LN - AH | 1.1 | 180 |
| ArC - LN - LC - AcO | 10.5 | 180 |
| ArC - AcC - AcO - HyO | 1.1 | 180 |
| ArC - AN - AH - AH | 1.1 | 180 |

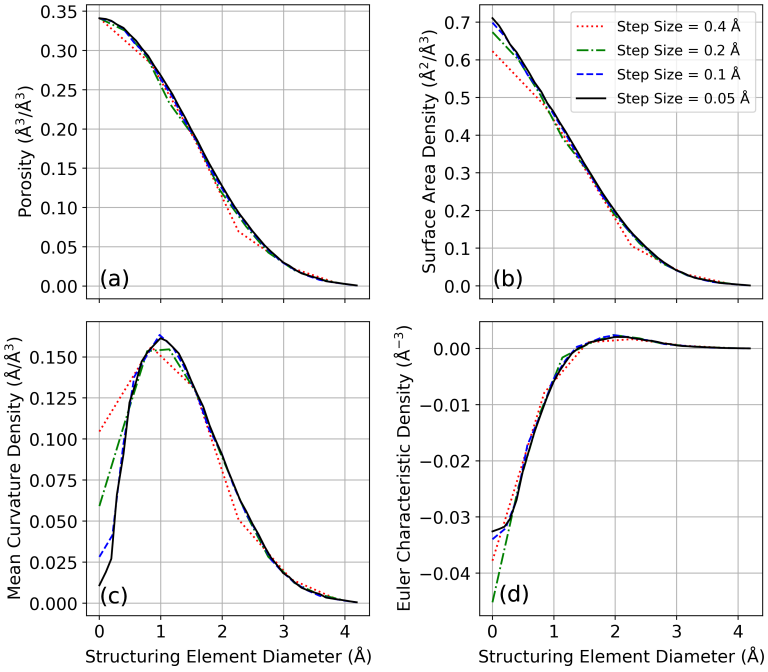


Figure S2: Minkowski functionals of dry, 1x domain pore space opening map: (a) free volume density, i.e. porosity; (b) free volume surface density; (c) mean free volume surface curvature density: (d) free volume Euler characteristic density.