



# New Efficient Adsorbent Materials for the Removal of Cd(II) from Aqueous Solutions

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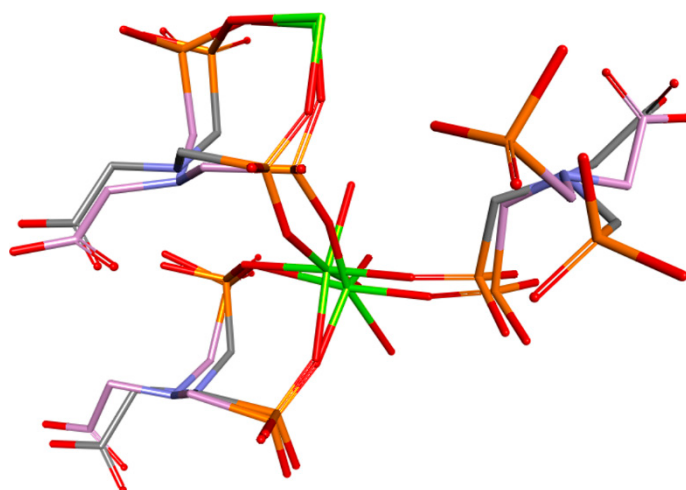


Figure S1. Superposition of the crystal structure of Mg-Gly (carbon atoms in grey) over the optimized structure of Mg-Gly (carbon atoms in purple) with PM3 semiempirical method. The RMSD between them is of 1.219 for heavy atoms.

Table S1. Geometric properties of the Mg-Gly model (CS - Crystal structure; OS - Optimized structure)

| Bond    | Distance |       |           | Bond Angle   | Degree  |         |           | Torsion Angle    | Degree   |          |           |
|---------|----------|-------|-----------|--------------|---------|---------|-----------|------------------|----------|----------|-----------|
|         | CS       | OS    | Residuals |              | CS      | OS      | Residuals |                  | CS       | OS       | Residuals |
| 57-O66  | 1.561    | 1.715 | -0.154    | O29-Mg56-O36 | 89.442  | 109.344 | -19.902   | C46-P25-O29-Mg56 | 66.587   | -24.389  | 90.976    |
| P57-O60 | 1.505    | 1.471 | 0.035     | Mg56-O36-P26 | 151.054 | 156.611 | -5.557    | P25-O29-Mg56-O36 | -77.663  | -2.868   | -74.795   |
| P57-C74 | 1.822    | 1.958 | -0.136    | O36-P26-C43  | 110.219 | 105.944 | 4.275     | O29-Mg56-O36-P26 | -30.074  | -10.206  | -19.868   |
| P2-O8   | 1.485    | 1.590 | -0.105    | P26-C43-N30  | 115.200 | 124.237 | -9.037    | Mg56-O36-P26-O32 | 147.757  | 118.695  | 29.062    |
| P2-O7   | 1.496    | 1.474 | 0.022     | C43-N30-C46  | 115.746 | 114.588 | 1.158     | O36-P26-O32-Mg27 | -36.196  | -123.688 | 87.492    |
| P2-O13  | 1.577    | 1.693 | -0.116    | N30-C46-P25  | 120.139 | 129.166 | -9.027    | P26-O32-Mg27-O4  | -82.983  | 24.247   | -107.230  |
| P26-O41 | 1.577    | 1.637 | -0.061    | C46-P25-O29  | 108.631 | 106.910 | 1.721     | P26-O32-Mg27-O8  | -171.513 | -56.855  | -114.658  |
| P26-O32 | 1.496    | 1.521 | -0.025    | P25-O29-Mg56 | 132.492 | 150.599 | -18.107   | P26-O32-Mg27-O33 | 12.571   | 100.428  | -87.857   |
| P26-C43 | 1.831    | 1.877 | -0.046    | O4-Mg27-O8   | 89.442  | 85.255  | 4.187     | P26-O32-Mg27-O65 | 99.401   | -167.967 | 267.368   |
| P25-O38 | 1.561    | 1.694 | -0.133    | O8-Mg27-O53  | 89.928  | 70.351  | 19.577    | O32-Mg27-O4-P1   | -178.943 | 172.126  | -351.069  |
| P25-O37 | 1.480    | 1.466 | 0.014     | O53-Mg27-O65 | 92.418  | 70.148  | 22.270    | O32-Mg27-O8-P2   | 55.192   | 35.097   | 20.095    |
| P1-O9   | 1.480    | 1.484 | -0.004    | O65-Mg27-O33 | 86.855  | 88.898  | -2.043    | Mg27-O8-P2-C15   | 23.384   | 33.866   | -10.482   |

|          |       |       |        |              |         |         |         |                  |          |         |          |
|----------|-------|-------|--------|--------------|---------|---------|---------|------------------|----------|---------|----------|
| P1-O10   | 1.561 | 1.724 | -0.163 | O33-Mg27-O32 | 89.632  | 109.699 | -20.067 | O4-Mg27-O8-P2    | -30.075  | -45.615 | 15.540   |
| P1-C18   | 1.822 | 1.959 | -0.137 | O32-Mg27-O4  | 85.465  | 84.555  | 0.910   | O32-Mg27-O65-P57 | -119.670 | 16.094  | -135.764 |
| O65-P57  | 1.505 | 1.471 | 0.035  | O4-Mg27-O53  | 89.329  | 105.720 | -16.391 | Mg27-O4-P1-C18   | 66.587   | 64.821  | 1.766    |
| O53-H55  | 0.930 | 0.971 | -0.041 | O4-Mg27-O65  | 177.264 | 167.653 | 9.611   |                  |          |         |          |
| O53-H54  | 0.929 | 0.970 | -0.041 | O4-Mg27-O33  | 95.508  | 78.936  | 16.572  |                  |          |         |          |
| O4-P1    | 1.505 | 1.556 | -0.051 | O8-Mg27-O65  | 88.486  | 103.645 | -15.159 |                  |          |         |          |
| O36-P26  | 1.485 | 1.642 | -0.157 | O8-Mg27-O33  | 168.434 | 124.678 | 43.756  |                  |          |         |          |
| O33-H35  | 0.900 | 0.959 | -0.059 | O8-Mg27-O32  | 101.199 | 121.142 | -19.943 |                  |          |         |          |
| O33-H34  | 0.821 | 0.973 | -0.152 | O53-Mg27-O33 | 80.704  | 63.954  | 16.750  |                  |          |         |          |
| O32-Mg27 | 2.033 | 1.867 | 0.167  | O53-Mg27-O32 | 168.544 | 165.792 | 2.752   |                  |          |         |          |
| N5-C15   | 1.504 | 1.493 | 0.011  | O65-Mg27-O32 | 93.183  | 97.732  | -4.549  |                  |          |         |          |
| N30-C46  | 1.511 | 1.521 | -0.010 |              |         |         |         |                  |          |         |          |
| Mg56-O36 | 2.023 | 1.789 | 0.234  |              |         |         |         |                  |          |         |          |
| Mg56-O29 | 2.088 | 1.804 | 0.285  |              |         |         |         |                  |          |         |          |
| Mg27-O8  | 2.023 | 1.861 | 0.163  |              |         |         |         |                  |          |         |          |
| Mg27-O65 | 2.018 | 1.876 | 0.143  |              |         |         |         |                  |          |         |          |
| Mg27-O53 | 2.145 | 2.479 | -0.334 |              |         |         |         |                  |          |         |          |
| Mg27-O4  | 2.088 | 2.500 | -0.412 |              |         |         |         |                  |          |         |          |
| Mg27-O33 | 2.113 | 1.891 | 0.222  |              |         |         |         |                  |          |         |          |

|         |       |       |        |
|---------|-------|-------|--------|
| C46-P25 | 1.822 | 1.918 | -0.097 |
| C43-N30 | 1.504 | 1.499 | 0.005  |
| C18-N5  | 1.511 | 1.500 | 0.012  |
| C15-P2  | 1.831 | 1.952 | -0.121 |

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