High accuracy geometric analysis of crystalline porous materials

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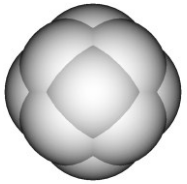
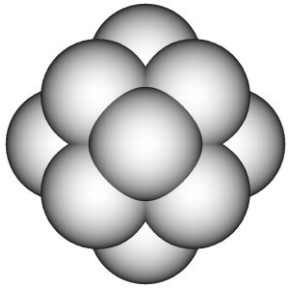
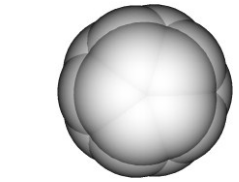
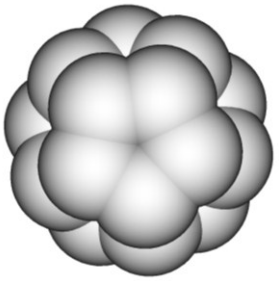
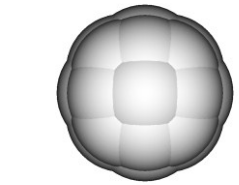
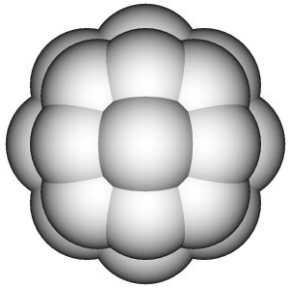
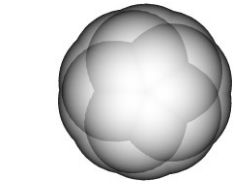
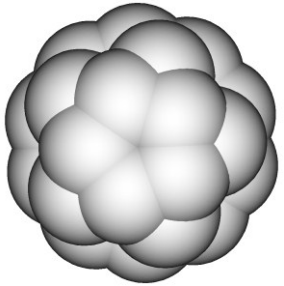
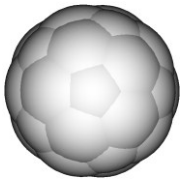
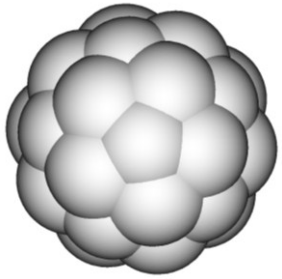
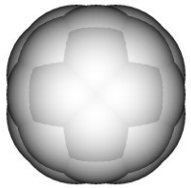
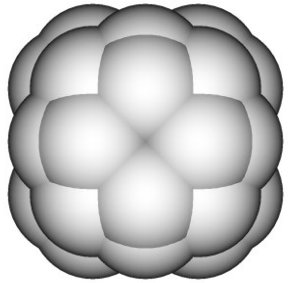
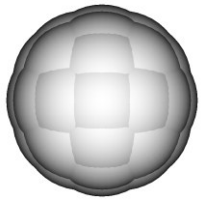
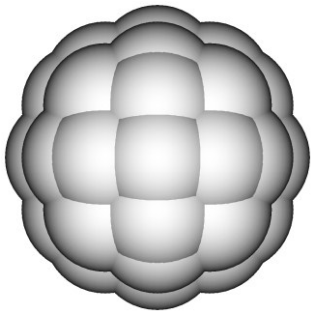
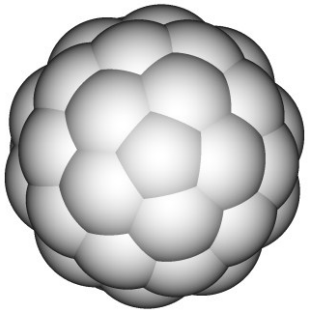
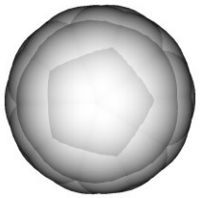
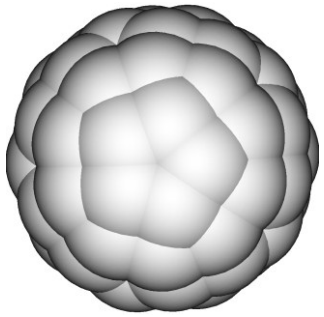
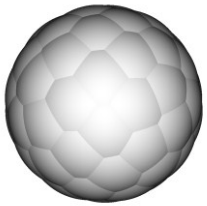
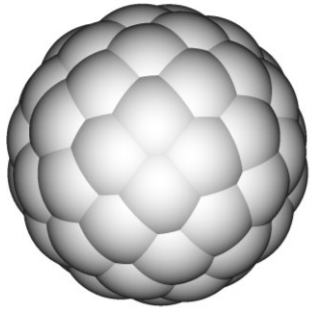
Supporting Information File

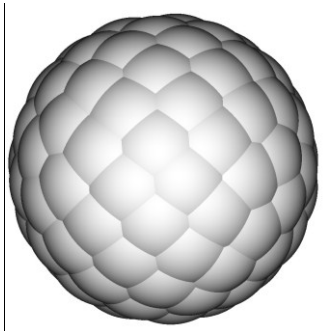
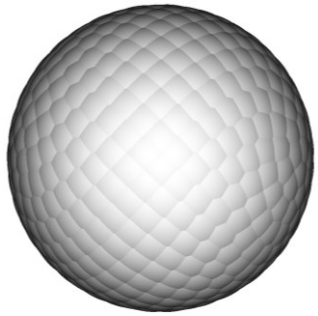
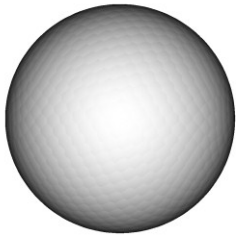
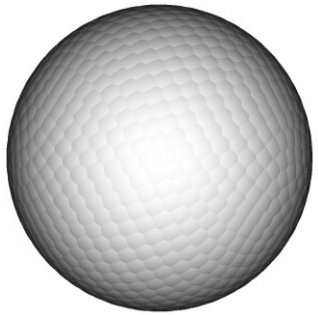
Clusters of small spheres are used to approximate the shape of larger spheres. This document provides details on accuracy of the approximation. A number of clusters based on polyhedrons (OCC, DDH, AQC, ICH, TIH, FCC, ACC, ICC, RIH) and Vogel spiral approximation (S60, S100, S500, S1000) are considered. We consider two scenario relevant to chemical systems:. A sphere of radius of 1.7A (e.g. carbon atom) and a sphere of radius of 2.7A (the largest radius in CCDC set). In both cases they are replaced with clusters of spheres of radius of 1.1A (e.g. hydrogen atom). The quality of approximation is measured by surface area and volume (based on Monte Carlo sampling in Zeo++ code) and their deviation from the corresponding sphere of larger radius (analytical solution).

Code	Name	Description	Type, Number of vertices	Shape approximation: R = 1.7A with 1.1A spherical probe	Reference sphere R = 1.7A SA: 98.47 A^2 Volume: 91.91 A^3	Shape approximation: R = 2.7A with 1.1A spherical probe	Reference sphere R = 2.7A SA: 181.37 A^2 Volume: 229.73 A^3
OCC	Octahedron + cube combination	Octahedron: regular polyhedron with 8 triangular faces Cube: All vertices at 45 degrees from xyz axes	Combination approximation 14 vertices + 1 center atom = 15 spheres		SA: 95.93 A^2 error: -2.98% Volume: 86.67 A^3 error: -5.70%		SA: 169.38 A^2 error: -6.61% Volume: 195.83 A^3 error: -14.76%

DDH	Dodecahedron	Polyhedron with 12 regular pentagonal faces	Polyhedron approximation 20 vertices + 1 center atom = 21 spheres		SA: 96.00 A^2 error: -2.51% Volume: 87.87 A^3 error: -4.40%		SA: 172.41 A^2 error: -4.94% Volume: 203.47 A^3 error: -11.43%
AQC	Axes + quadrant + cube combination	Axes: spheres with coordinates on all +- axes Quadrant: spheres placed at 45 degree position in xz, and yz axes Cube: All vertices at 45 degrees from xyz axes	Combination approximation 26 vertices + 1 center atom = 27 spheres		SA: 96.87 A^2 error: -1.62% Volume: 88.96 A^3 error: -3.21%		SA: 174.62 A^2 error: -3.72% Volume: 210.27 A^3 error: -8.48%
ICH	Icosidodeca-hedron	Polyhedron with 20 triangular and 12 regular pentagonal faces	Polyhedron approximation 30 vertices + 1 center atom = 31 spheres		SA: 96.43 A^2 error: -2.07% Volume: 89.24 A^3 error: -2.90%		SA: 174.43 A^2 error: -3.82% Volume: 212.08 A^3 error: -7.68%

TIH	Truncated isohedron	Polyhedron with 12 regular pentagonal faces and 20 regular hexagonal faces. Corresponds to DDH with spheres placed at face centers.	Polyhedron approximation 32 vertices + 1 center atom = 33 spheres		SA: 96.39 A^2 error: -2.11% Volume: 88.83 A^3 error: -3.35%		SA: 174.12 A^2 error: -3.99% Volume: 210.63 A^3 error: -8.32%
FCC	Four cubes combination	1 cube with vertices 45 degrees with respect to xyz axes, 1 cube with vertices along xy axes, 1 cube with vertices along xz axes, 1 cube with vertices along yz axes.	Combination approximation 32 vertices + 1 center atom = 33 spheres		: 96.30 A^2 or: -2.21% lume: 88.98 A^3 or: -3.18%		SA: 174.29 A^2 error: -3.90% Volume: 210.53 A^3 error: -8.36%
ACC	Axis + cubes combination	FCC structure with the addition of spheres with coordinates along all +- axes	Combination approximation 38 vertices + 1 center atom = 39 spheres		: 96.85 A^2 or: -1.65% lume: 89.79 A^3 or: -2.30%		SA: 176.13 A^2 error: -2.89% Volume: 215.49 A^3 error: -6.20%

ICC	Icosidodeca-hedron + center spheres combination	ICH structure with 12 additional spheres corresponding to the center of the pentagonal faces	Combination approximation 42 vertices + 1 center atom = 43 spheres		.: 96.98 A^2 or: -1.51% lume: 90.19 A^3 or: -1.87%		SA: 176.85 A^2 error: -2.49% Volume: 218.13 A^3 error: -5.05%
RIH	Rhombicosi-dodecahedron	Polyhedron with 20 regular triangular faces, 30 square faces, and 12 regular pentagonal faces.	Polyhedral approximation 60 vertices + 1 center atom = 61 spheres		: 97.61 A^2 or: -0.87% lume: 90.65 A^3 or: -1.37%		SA: 178.33 A^2 error: -1.67% Volume: 221.11 A^3 error: -3.75%
S60	60 sphere spiral	60 spheres generated in a spiral	Spiral approximation 60 vertices + 1 center atom = 61 spheres		SA: 98.37 error: -0.10% Volume: 90.70 error: -1.31%		SA: 179.56 error: -1.00% Volume: 224.38 error: -3.63%

S100	100 sphere spiral	100 spheres generated in a spiral	Spiral approximation 100 vertices + 1 center atom = 101 spheres		SA: 98.80 error: 0.33% Volume: 91.22 error: -0.75%		SA: 180.45 error: -0.51% Volume: 224.78 error: -2.16%
S500	500 sphere spiral	500 spheres generated in a spiral	Spiral approximation 500 vertices + 1 center atom = 501 spheres		SA: 98.42 error: -0.05% Volume: 91.82 error: -0.09%		SA: 181.37 error: -0.12% Volume: 228.91 error: -0.36%
S1000	1000 spheres	1000 spheres generated in a spiral	Spiral approximation 1000 vertices + 1 center atom = 1001 spheres		SA: 98.47 error: -0.03% Volume: 91.90 error: -0.003%		SA: 181.35 error: -0.01% Volume: 229.44 error: -0.13%