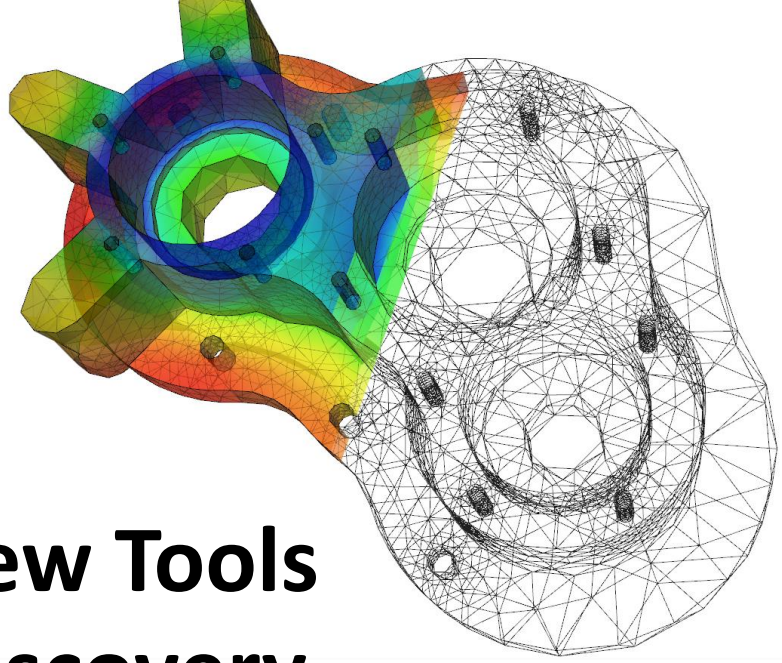


The Need for New Tools for Materials Discovery

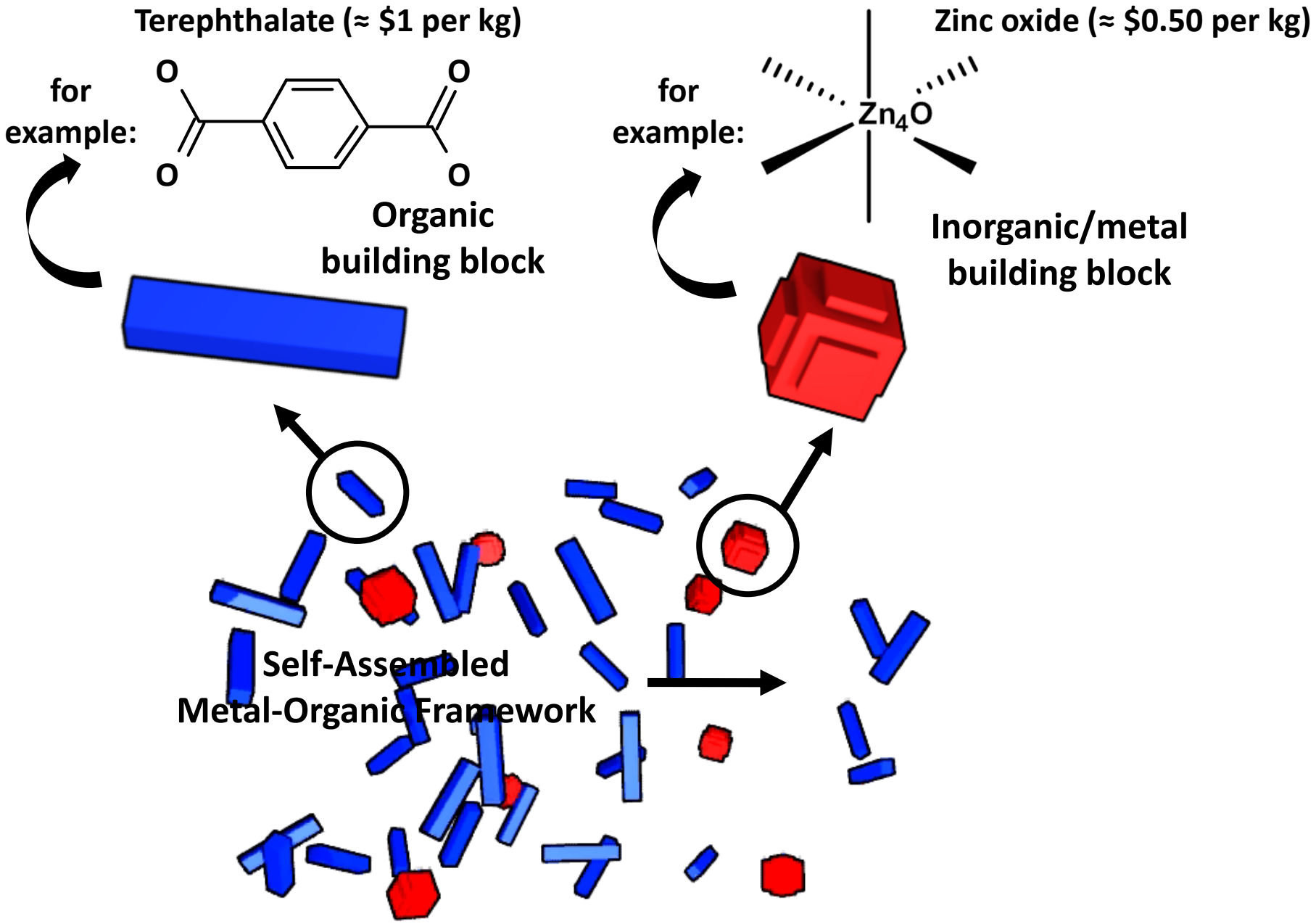
Kutay Sezginel, Paul Boone, Christopher E. Wilmer

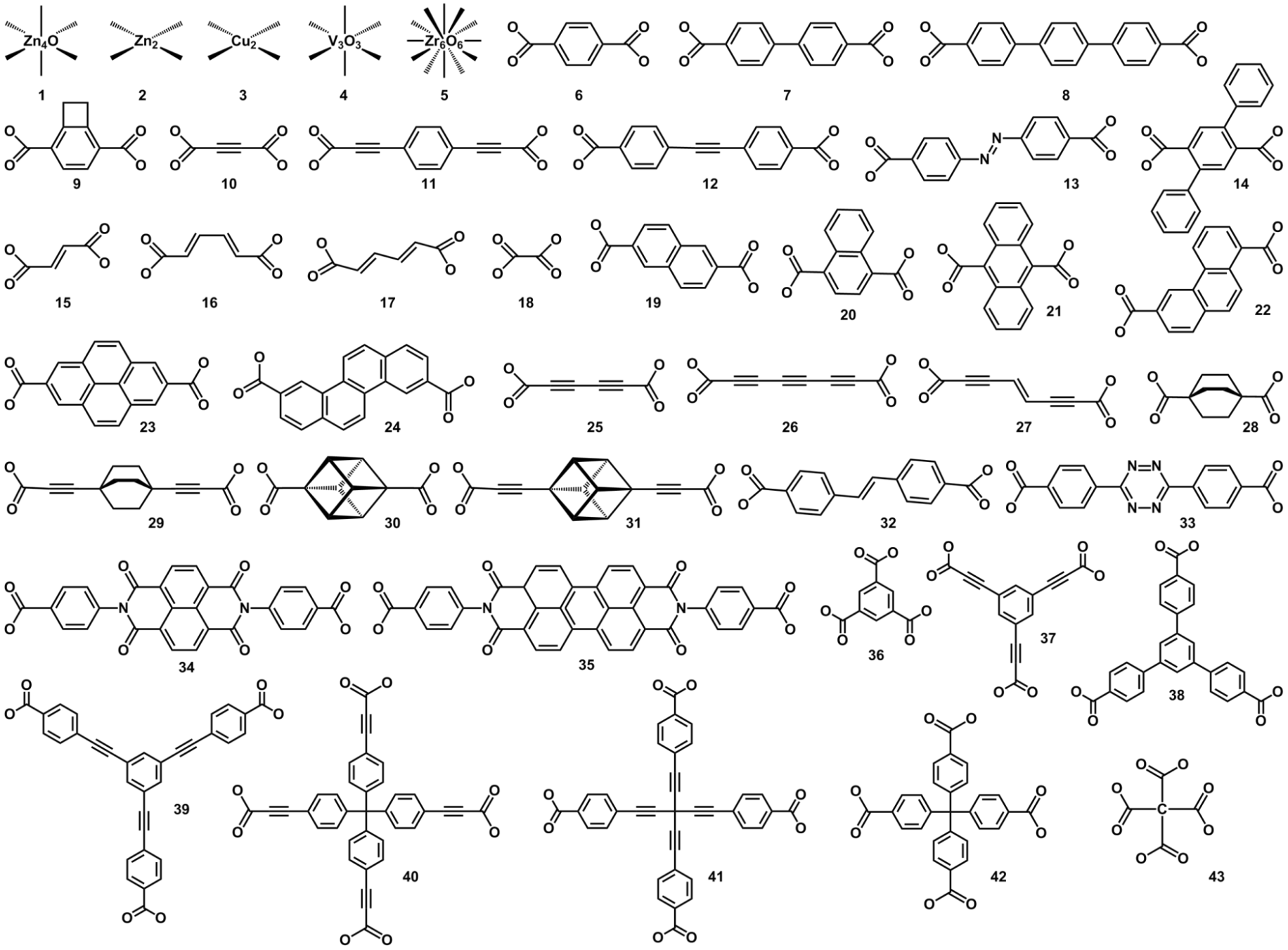
www.wilmerlab.com

Dept. of Chemical & Petroleum Engineering
University of Pittsburgh

Talk Outline

- A recent (small) materials discovery problem:
  - Simulating hypothetical “MOF” structures
- A much bigger materials discovery problem
- Our vision for the tools needed for solving it


Terephthalate (≈ $1 per kg)
for example:
O
O
O
O
Organic building block
Zinc oxide (≈ $0.50 per kg)
for example:
Zn_4O
Inorganic/metal building block
Self-Assembled Metal-Organic Framework


Zn4O
Zn2
Cu2
V3O3
Zr6O6
1
2
3
4
5
6
7
8
9
10
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12
13
14
15
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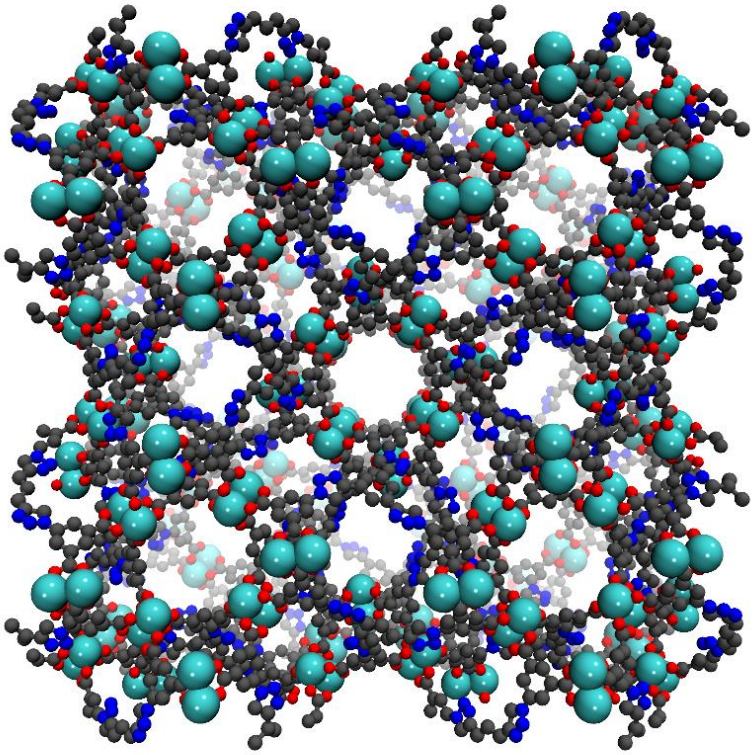
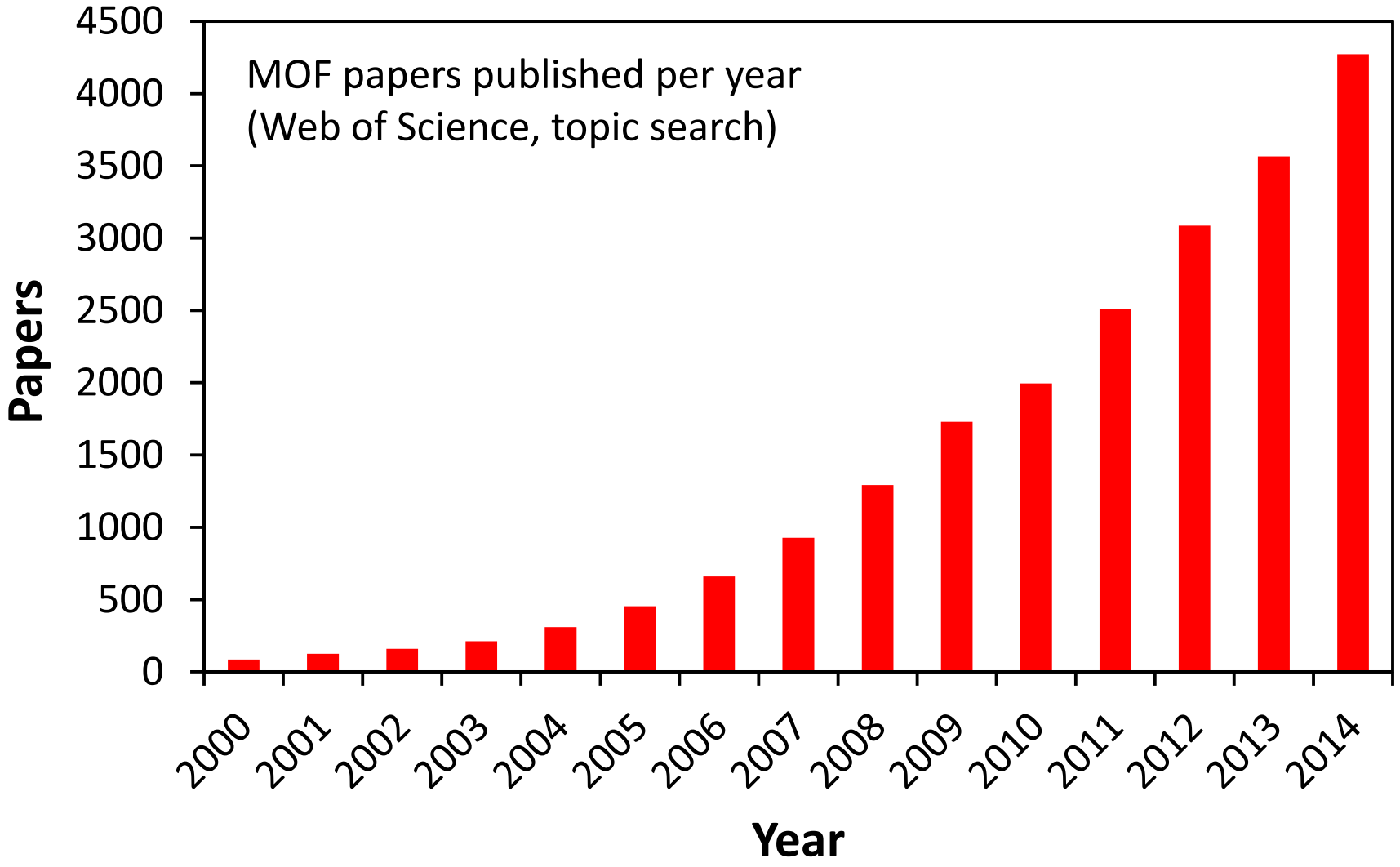
Applications of MOFs

- Better natural gas fuel tanks
- CO_2 capture
- Hydrogen storage
- Oxygen storage
- Gas masks
- Gas sensors
- Etc.

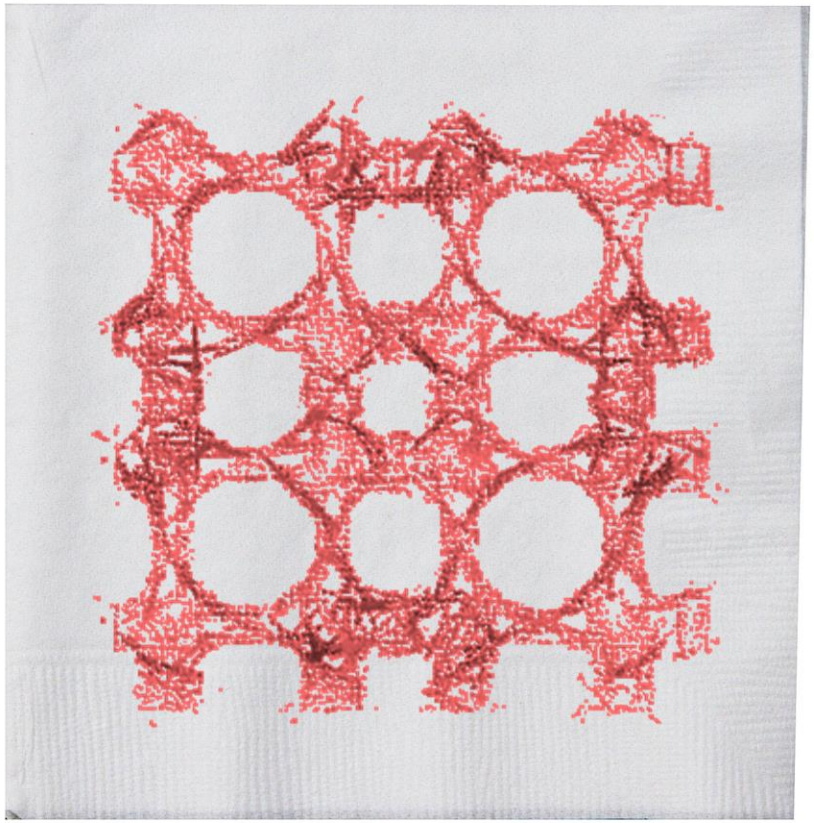


Explosion of papers on MOFs

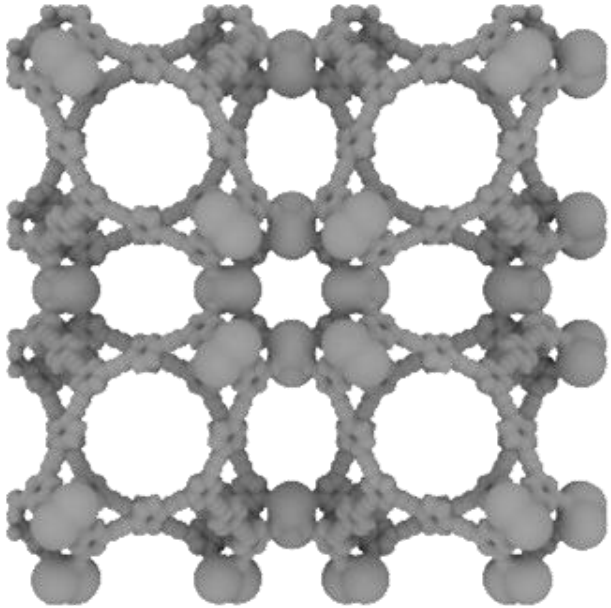


MOF design, circa 2000

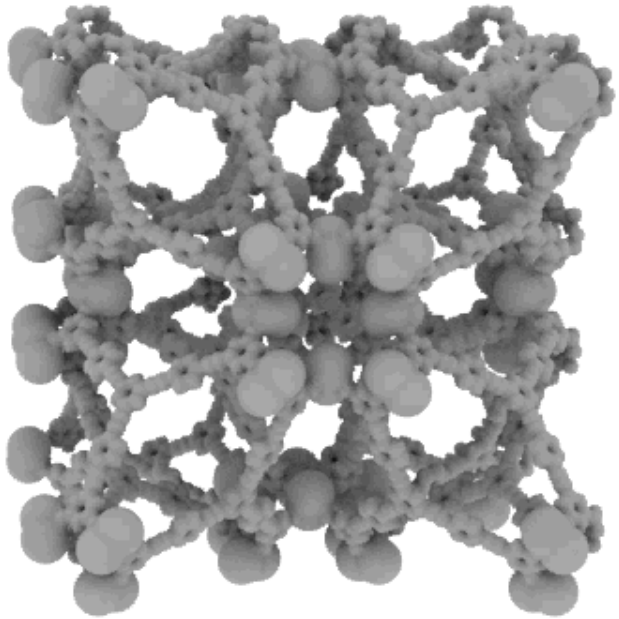
1. Draw proposed MOF structure on napkin (or whiteboard)



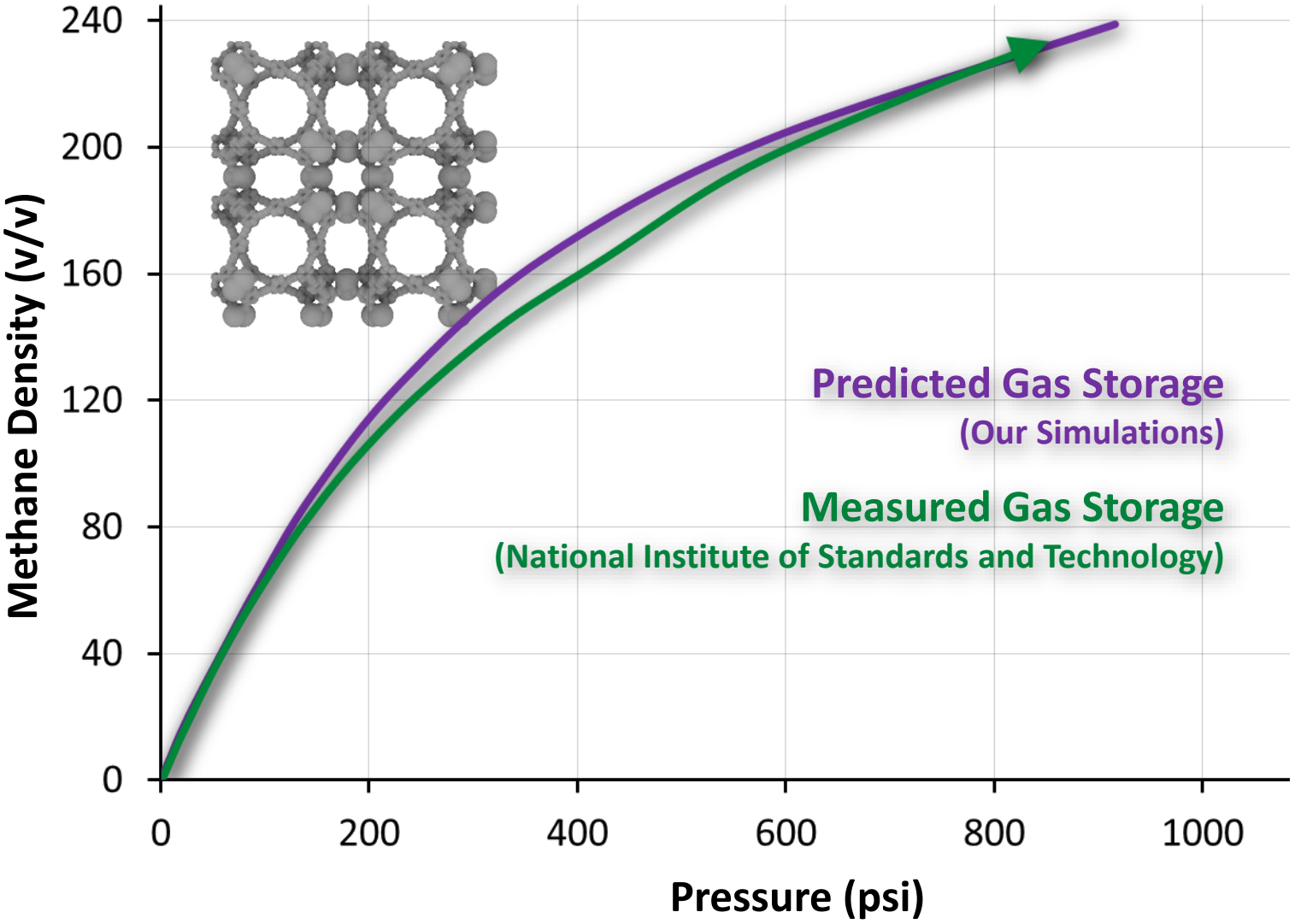
2. Create actual MOF structure in the chemistry lab



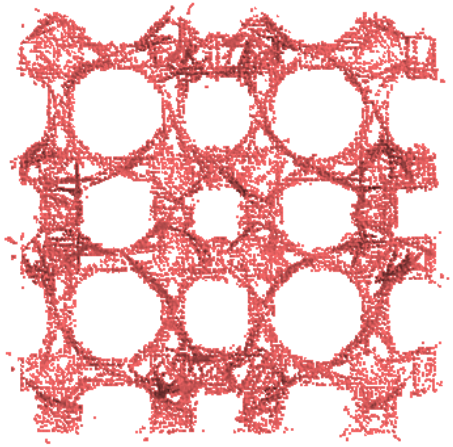
Step 3.
Predict properties using molecular simulations



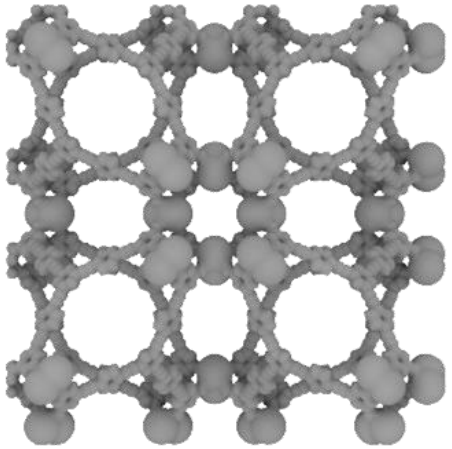
Predictions can be pretty accurate!

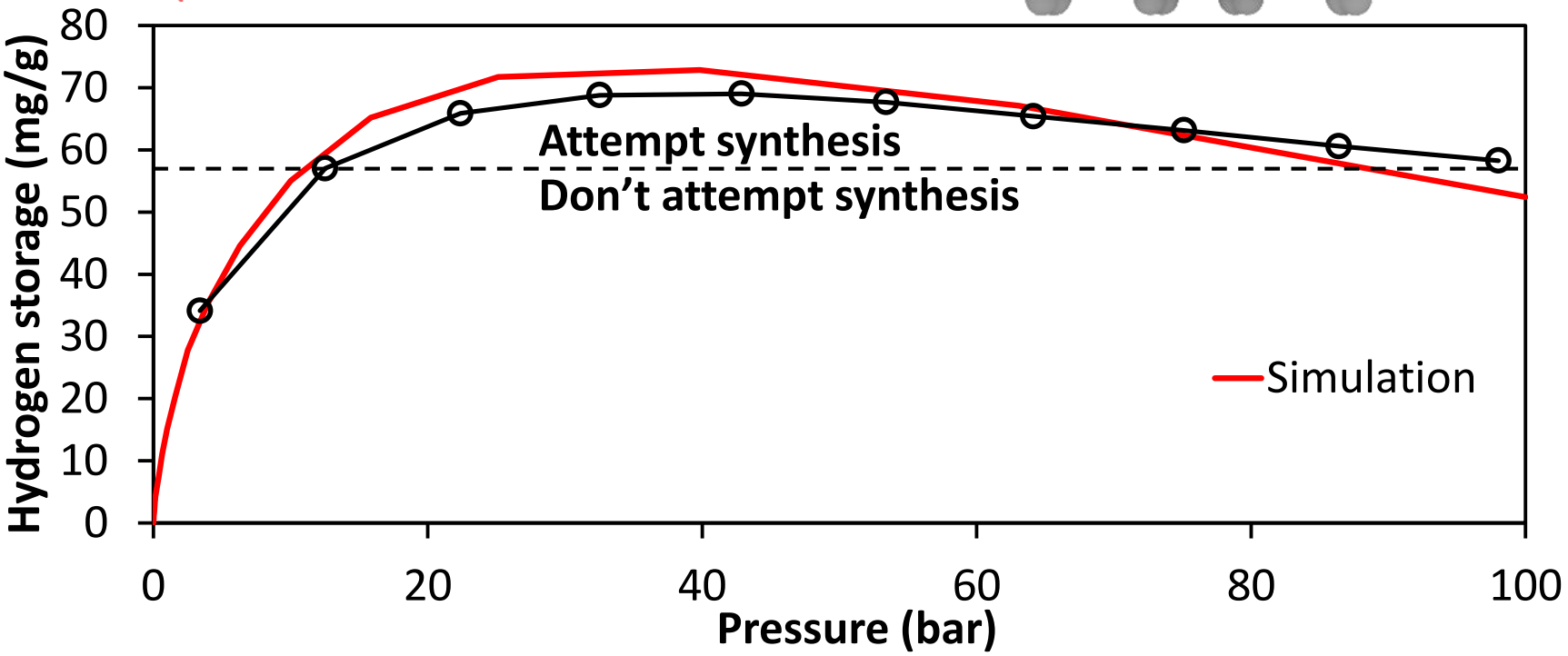


A glaring inefficiency…



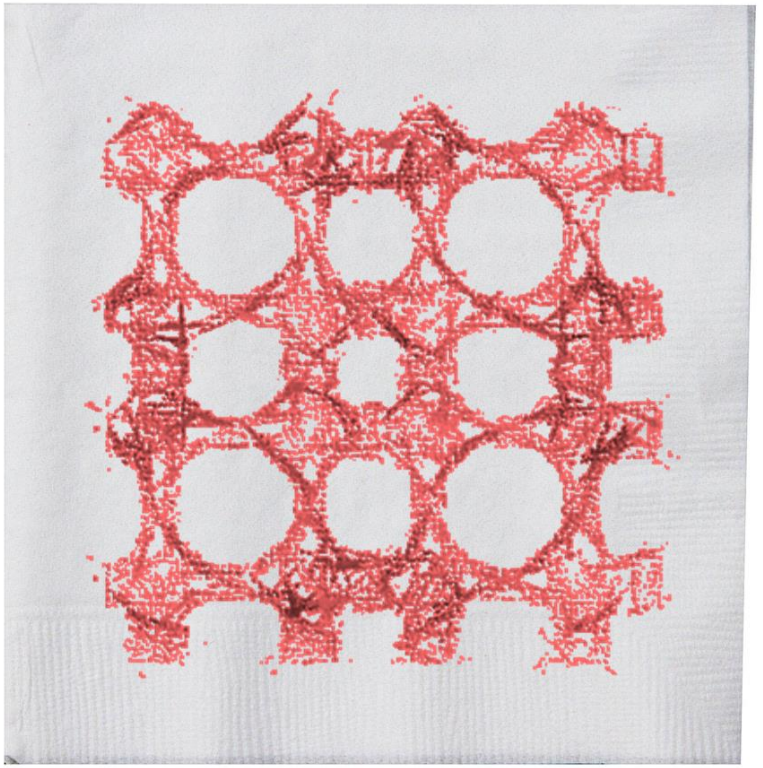
Expensive
Takes “months”



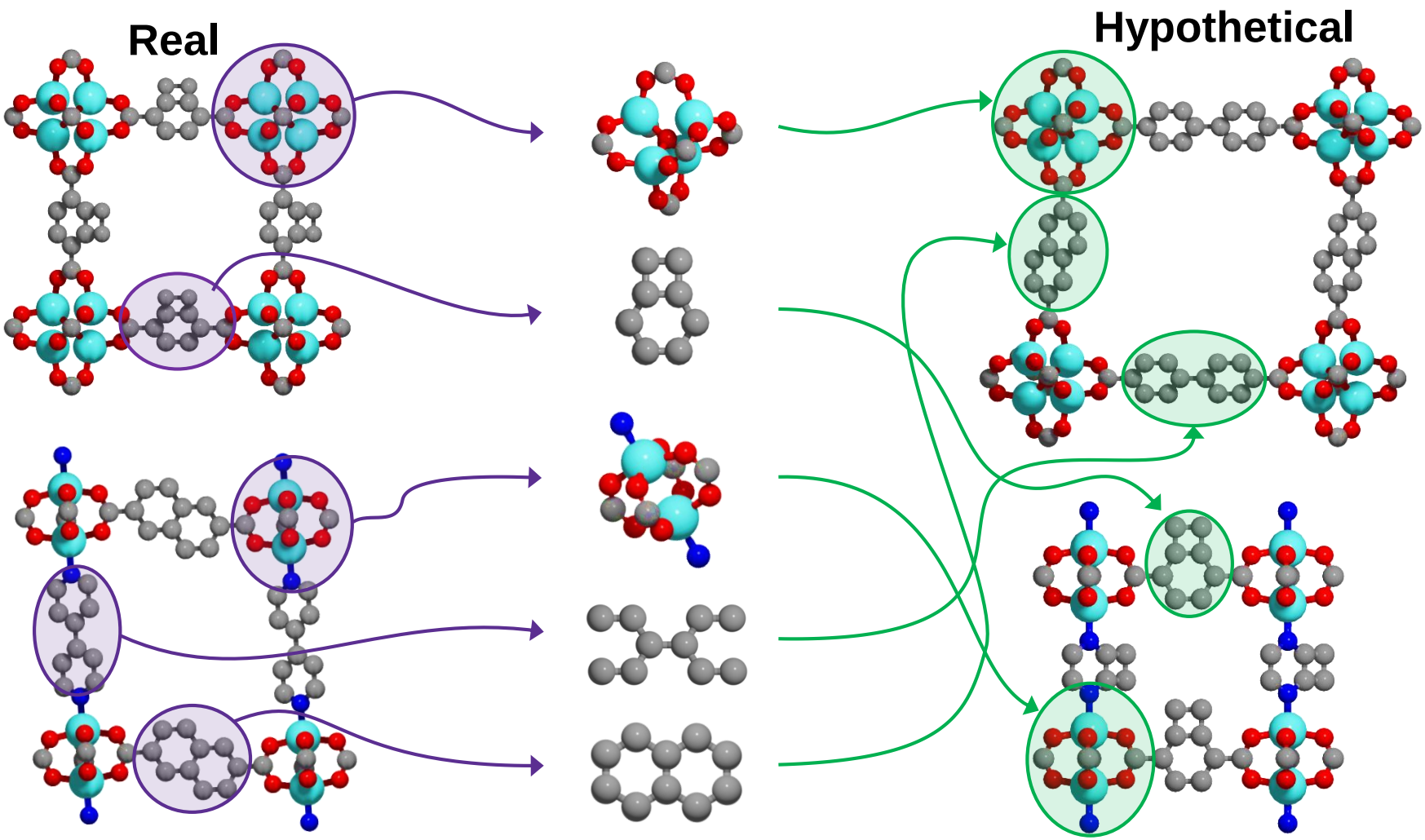


No tools for drawing MOFs on a computer!

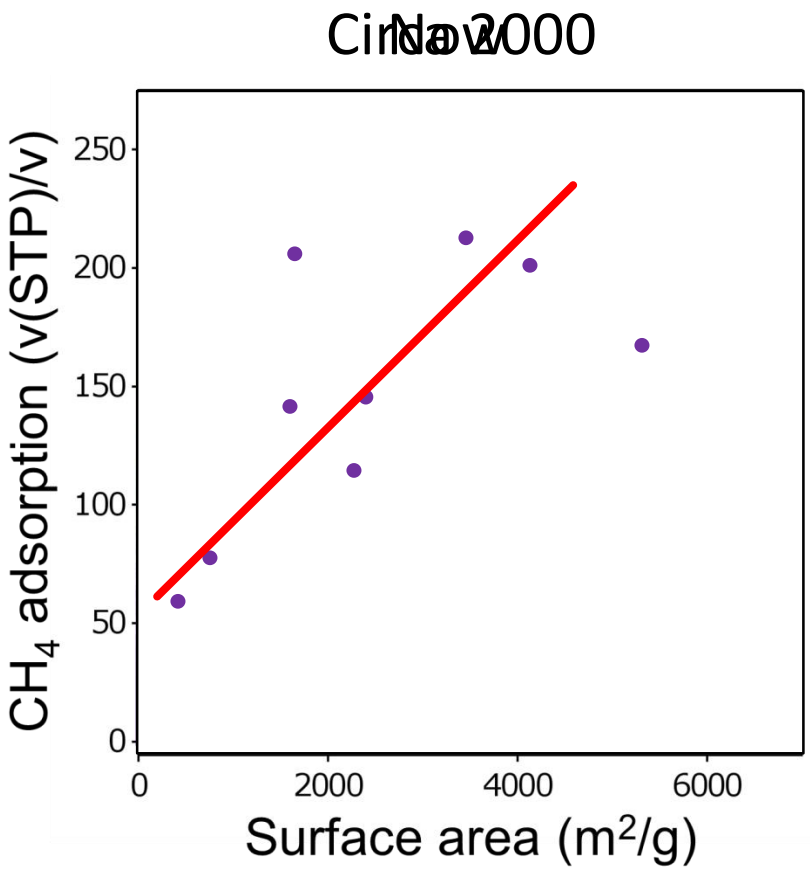
- State of the art was napkins and whiteboards
- Existing chemical drawing/building programs were slow, impractical; typical MOFs had 1000s of atoms, 3d structures, etc.
- No automation capability
- Bottleneck meant experimentalists were always leading and computationalists following

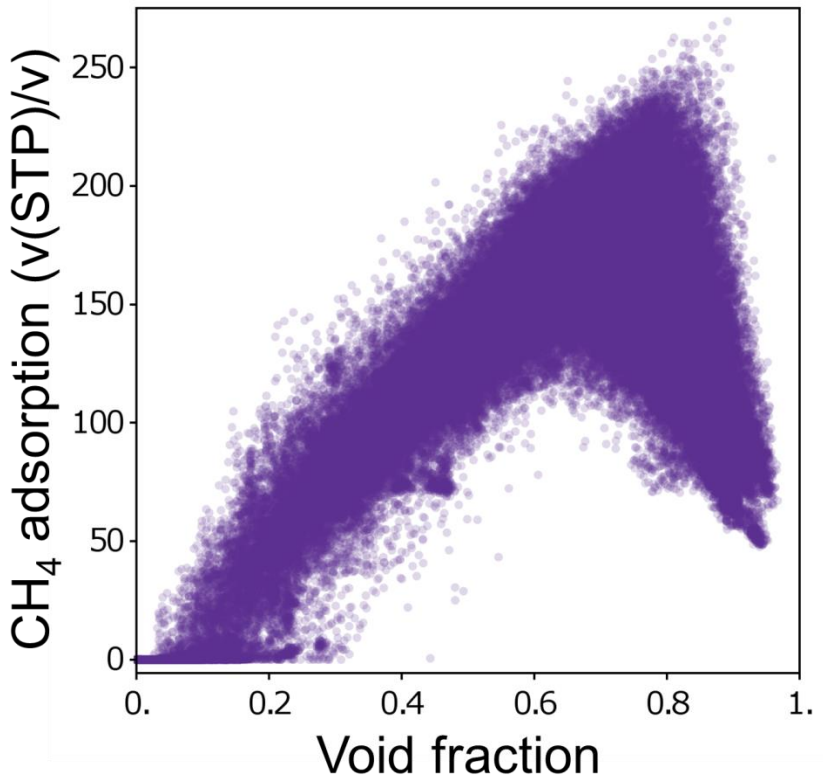


Generating Hypothetical MOFs

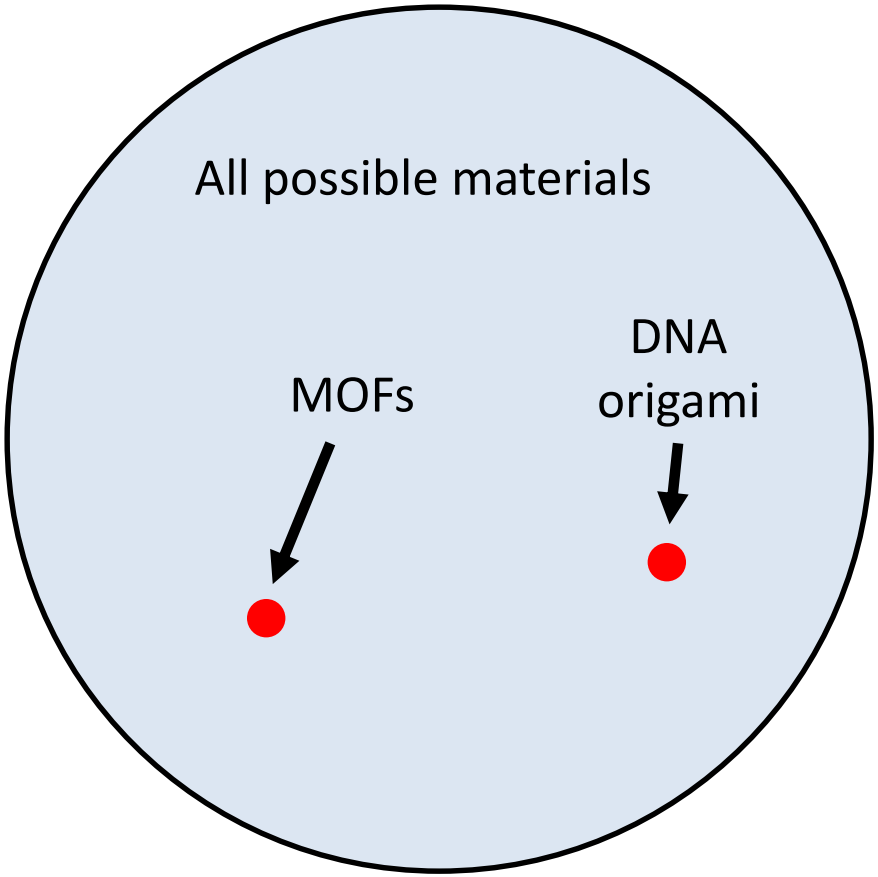


Benefits of having a tool for exploring hypothetical MOFs

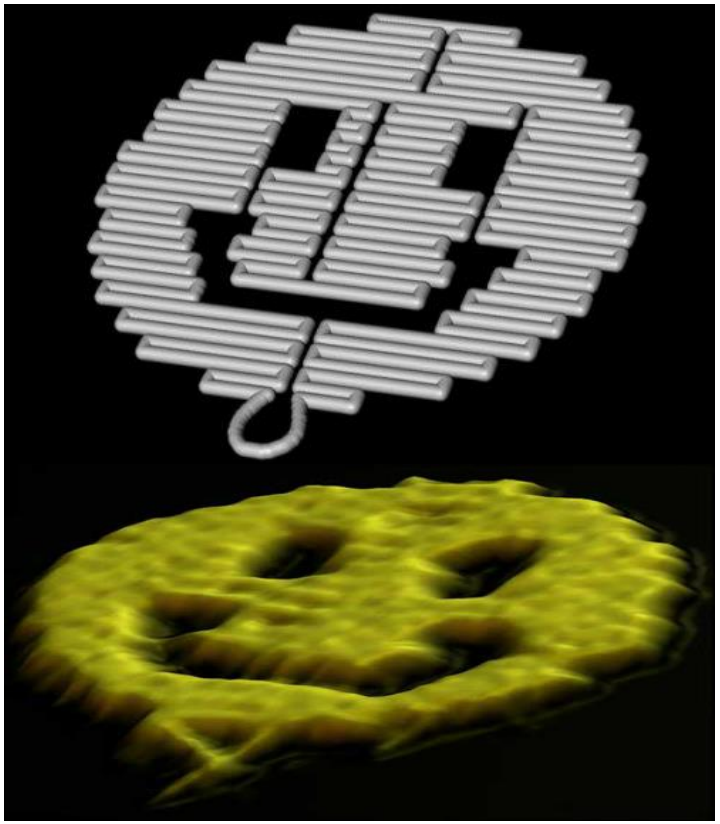


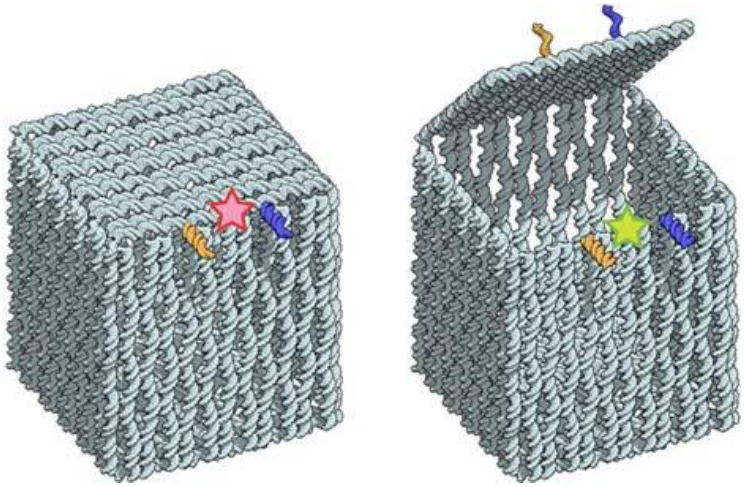


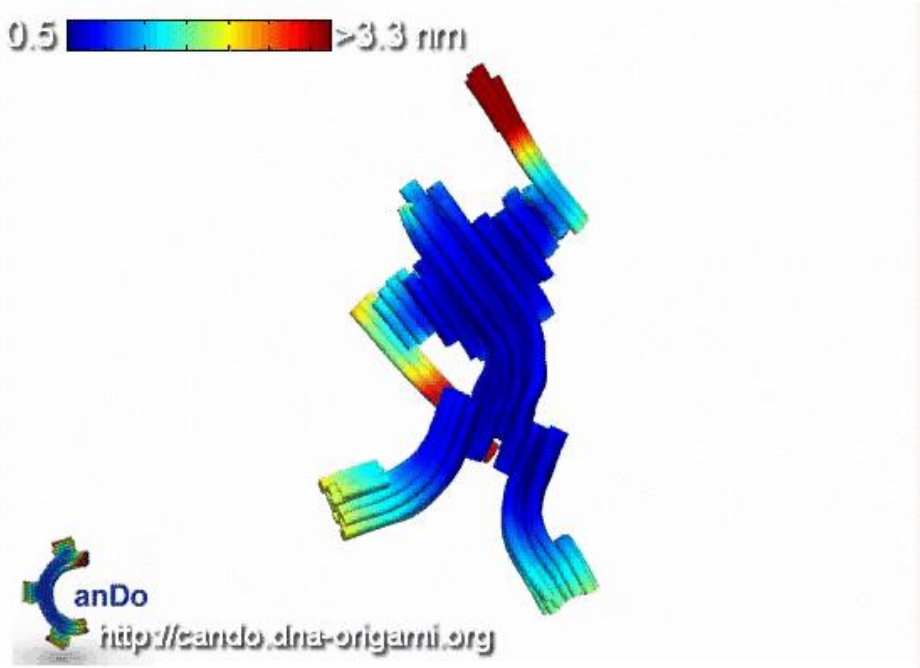
Generating hypothetical MOFs is a small dent in a much bigger materials discovery problem



CADnano
A CAD tool for DNA origami-based structures







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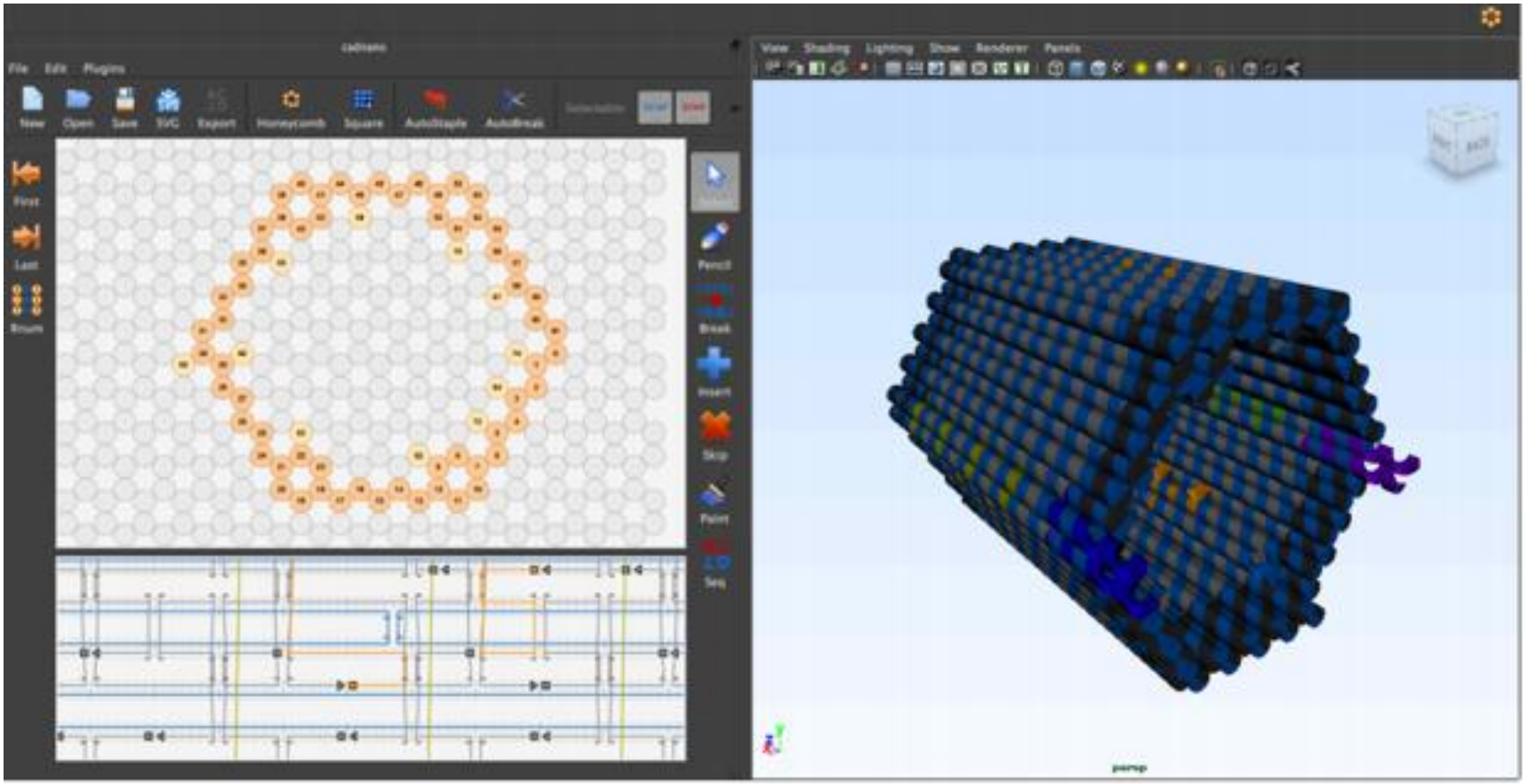
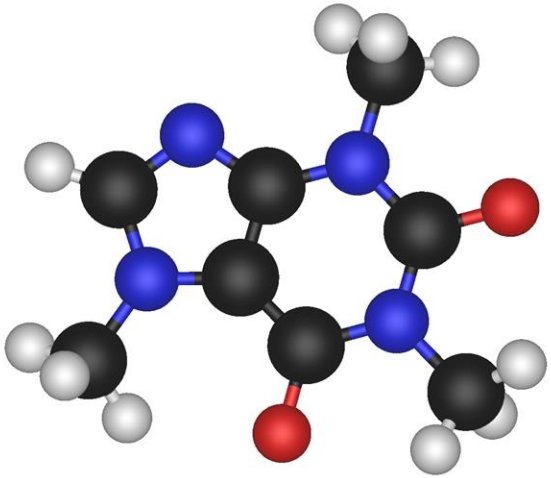


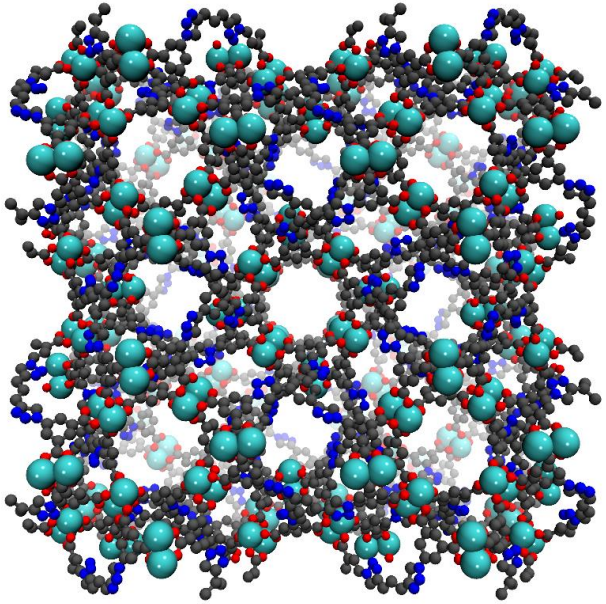
"For small systems humans have been able to manually construct trial molecular configurations…

…however, for systems involving thousands of atoms creating trial configurations is much more challenging."

The Need for New Tools for Materials Discovery

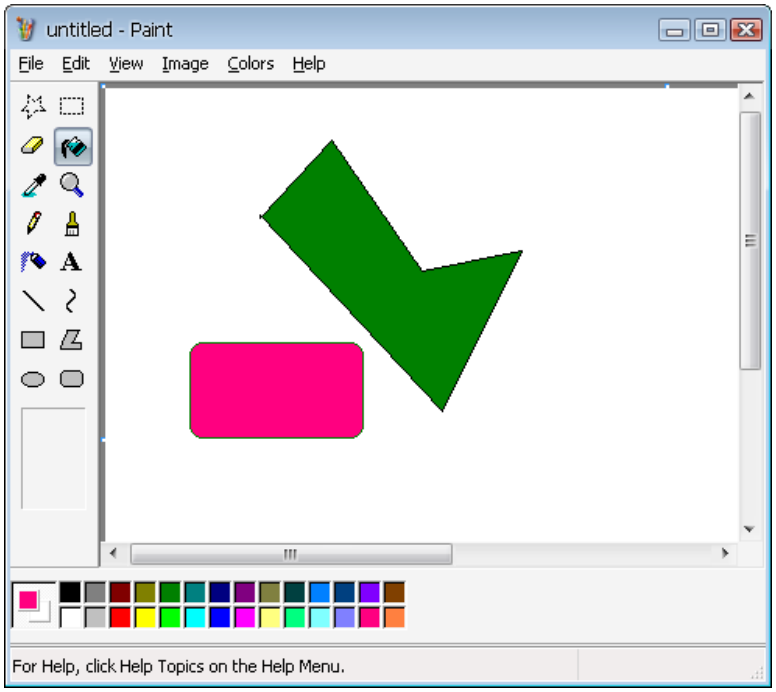


(need better "drawing" tools for molecular systems)

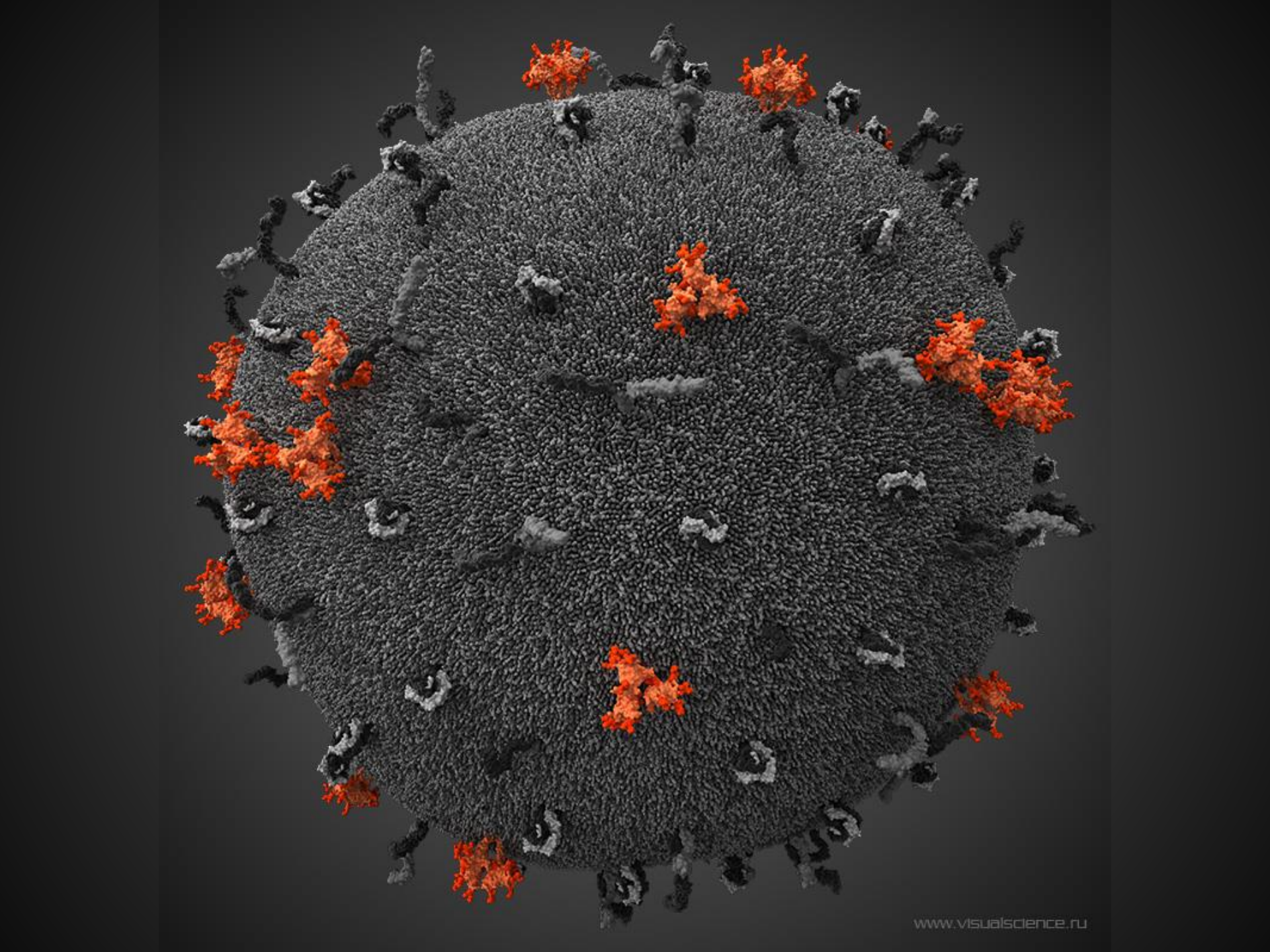


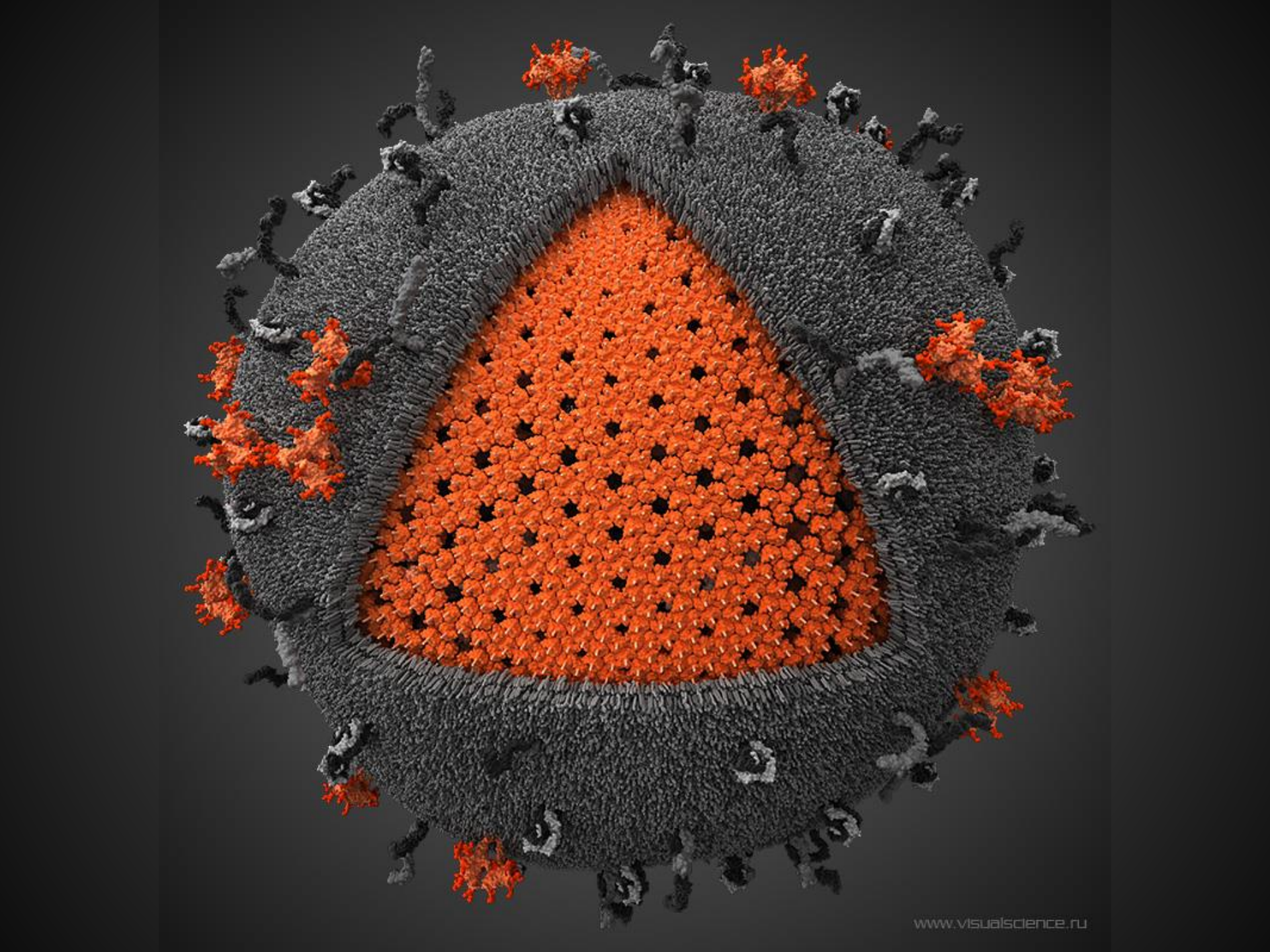
Existing chemical drawing tools are very limited for generating complex molecular systems

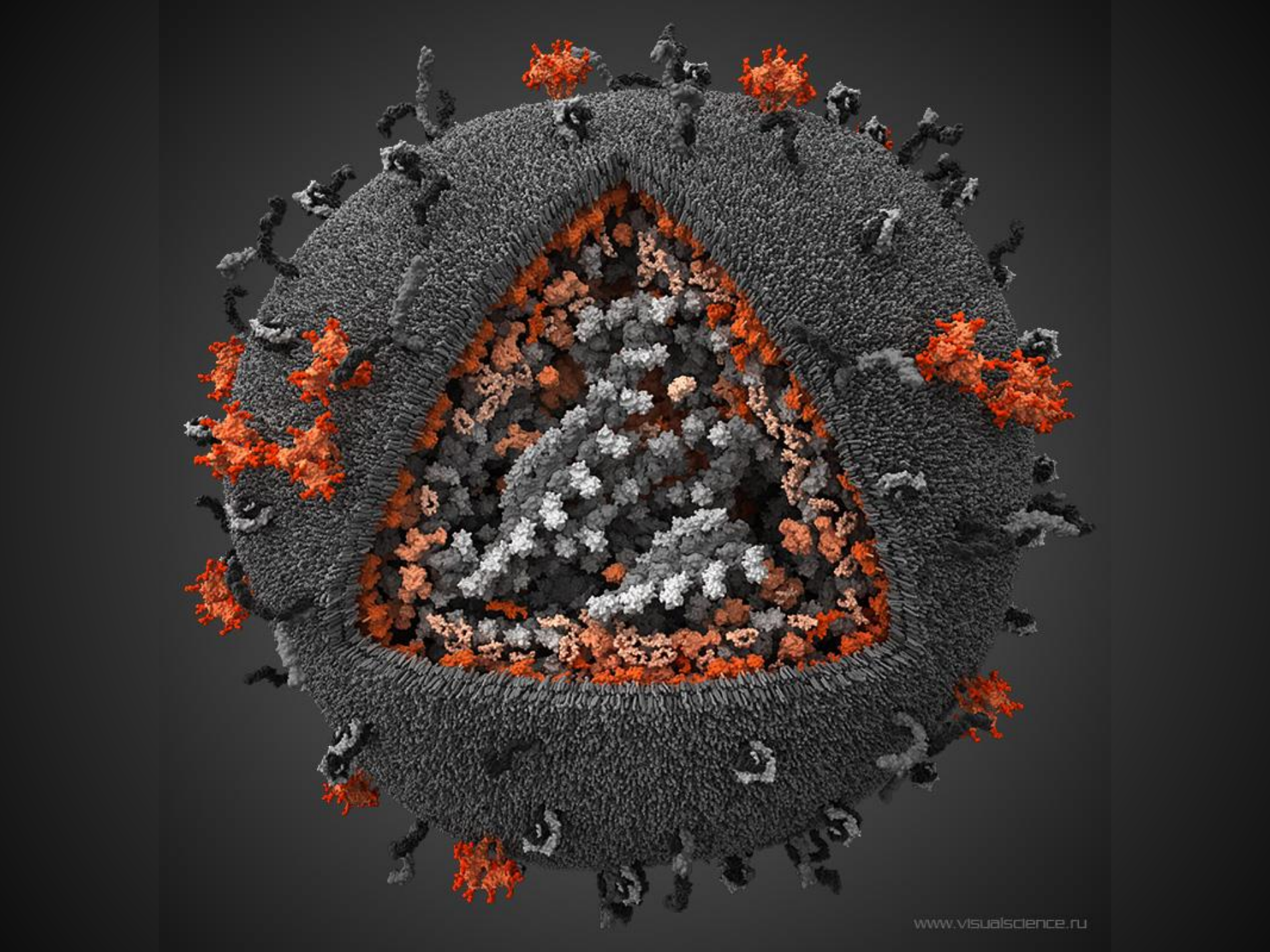
Microsoft Paint

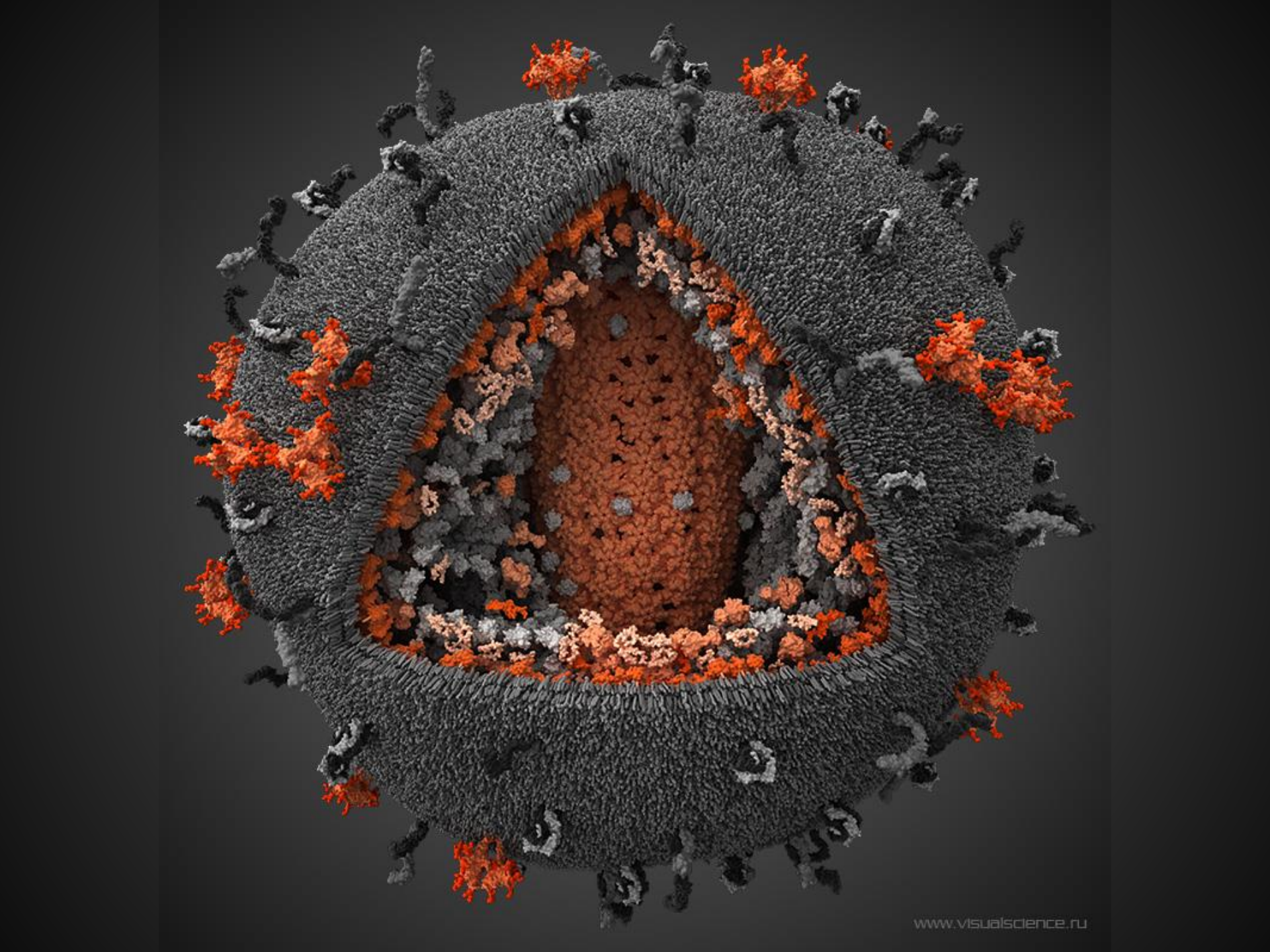


Internal Combustion Engine


www.visualscience.ru


www.visualscience.ru


www.visualscience.ru


www.visualscience.ru

My (abbreviated) wish list of features for a molecular CAD program:

- Handle hundreds of thousands of atoms
- Easily fill any “standard” geometric volume (sphere, cylinder, tetrahedron, etc.) with a predefined pattern/motif
- Provide standard CAD geometry building tools (extrusion, lathing, arrays)
- Boolean operations on structures (union, intersection, diff.)
- Smart geometry modifiers (scaling, shearing, twisting, etc.)
- (all) Point group symmetry constraints available when building 0-d structures
- (all) Space group symmetry constrains for building periodic structures
- Building larger structures from smaller structures
- Generating trial trajectories with inverse kinematics