

# BetaCavity: Program for Molecular Voids and Tunnels

**Jae-Kwan Kim<sup>1</sup>, Youngsong Cho<sup>1</sup>, Joonghyun Ryu<sup>1</sup>, Mokwon Lee<sup>2</sup>,  
Jehyun Cha<sup>2</sup>, Chanyoung Song<sup>2</sup>, and Deok-Soo Kim<sup>1,2</sup>**

<sup>1</sup> Voronoi Diagram Research Center, Hanyang University, Korea

<sup>2</sup> Dept. Mechanical Engineering, Hanyang University, Korea

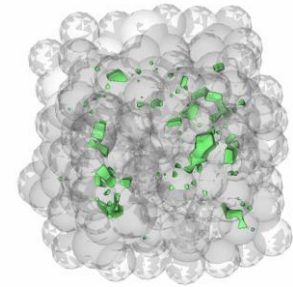
**September 29(Mon) - 30(Tue), 2014**

**The Eleventh Korea-US Nano Forum  
Seoul National University, Seoul, Korea**

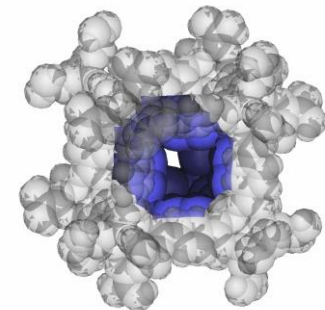
# BetaCavity

---

- A program for recognizing cavities (molecular of voids / tunnels)
- Functions
  - Mass properties of cavities (volume / boundary area)
  - Contributing area of each atoms
  - Other solution related with geometry
- Easy to use: GUI program for Windows (Linux version was also implemented)
- Download at VDRC website freely (<http://voronoi.hanyang.ac.kr/software>)



Voids in amorphous material



Tunnels in MOF

# Functions for Voids

**Cavities**

- Voids (sorted by void volume)
- Void 1 (vol: 0.650, area: 10.278)
- Void 2 (vol: 0.562, area: 5.791)
- Void 3 (vol: 0.538, area: 5.786)
- Void 4 (vol: 0.280, area: 4.623)
- Void 5 (vol: 0.277, area: 3.536)
- Void 6 (vol: 0.171, area: 3.338)
- Void 7 (vol: 0.166, area: 2.844)
- Void 8 (vol: 0.130, area: 2.315)
- Void 9 (vol: 0.116, area: 1.950)
- Void 10 (vol: 0.112, area: 2.798)
- Void 11 (vol: 0.075, area: 2.314)
- Void 12 (vol: 0.064, area: 1.142)
- Void 13 (vol: 0.055, area: 2.032)
- Void 14 (vol: 0.049, area: 1.971)
- Void 15 (vol: 0.048, area: 1.202)
- Void 16 (vol: 0.042, area: 1.767)
- Void 17 (vol: 0.037, area: 1.098)
- Void 18 (vol: 0.034, area: 0.810)
- Void 19 (vol: 0.031, area: 1.621)
- Void 20 (vol: 0.031, area: 0.781)
- Void 21 (vol: 0.030, area: 0.900)
- Void 22 (vol: 0.022, area: 0.712)
- Void 23 (vol: 0.021, area: 0.861)

**Properties**

**VOID 1**

- Mass properties
- Volume of voids: 0.650
- Area of voids: 10.278

Contributing atoms (+ area, charge, hydrophc)

ATOM	Residue	MOL	Count	Area	Charge	Hydrophc
173	NI73	MOL	2	29.033 A <sup>2</sup>	0	0
161	NI61	MOL	2	29.033 A <sup>2</sup>	0	0
206	P6	MOL	2	40.715 A <sup>2</sup>	0	0
213	P13	MOL	2	40.715 A <sup>2</sup>	0	0
111	NI11	MOL	2	29.033 A <sup>2</sup>	0	0
105	NI5	MOL	2	29.033 A <sup>2</sup>	0	0
65	Pd65	MOL	2	29.033 A <sup>2</sup>	0	0
40	Pd40	MOL	2	29.033 A <sup>2</sup>	0	0
50	Pd50	MOL	2	29.033 A <sup>2</sup>	0	0
42	Pd42	MOL	2	29.033 A <sup>2</sup>	0	0
52	Pd52	MOL	2	29.033 A <sup>2</sup>	0	0
28	Pd28	MOL	2	29.033 A <sup>2</sup>	0	0
25	Pd25	MOL	2	29.033 A <sup>2</sup>	0	0
19	Pd19	MOL	2	29.033 A <sup>2</sup>	0	0
16	Pd16	MOL	2	29.033 A <sup>2</sup>	0	0

**VOID 2**

- Mass properties
- Volume of voids: 0.562
- Area of voids: 5.791

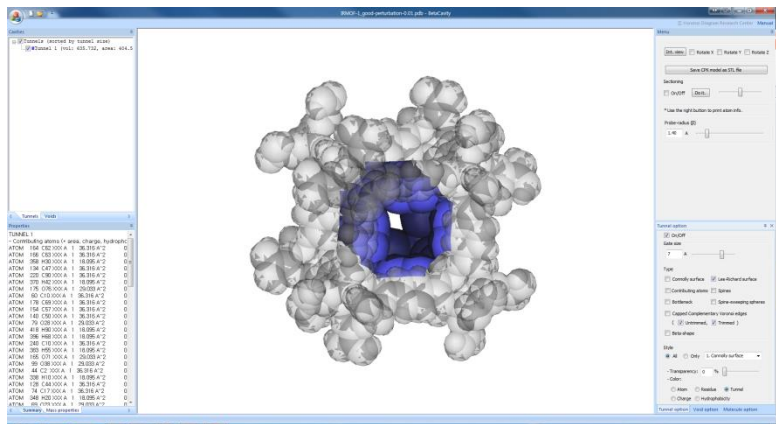
**Menu**

- Int. view
- Rotate X
- Rotate Y
- Rotate Z
- Save CPK model as STL file
- Sectioning: On/Off
- Probe-radius (R): 0.2 A

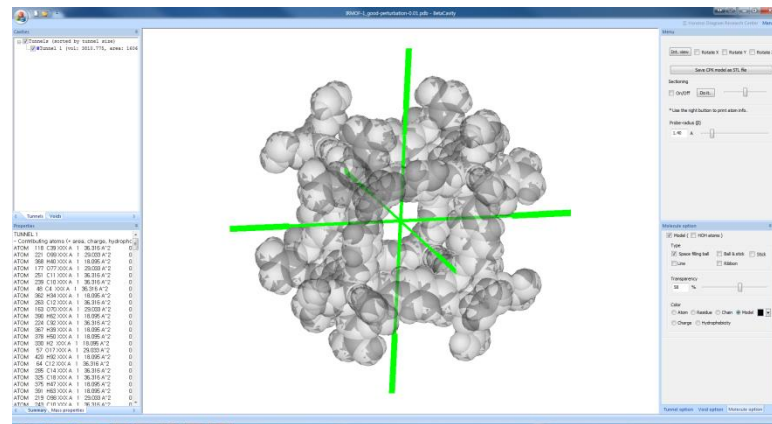
**Void option**

- On/Off
- Type: Connolly surface, Lee-Richard surface, Contributing atoms, Spines, Complementary Voronoi edges, Beta-shape
- Style: All, Only, 3. Contributing atoms
- Transparency: 30%
- Color: Atom, Residue, Tunnel, Charge, Hydrophobicity
- Filter: Void volume > 0.0 A<sup>3</sup>, Void area > 0.0 A<sup>2</sup>, Voids with spine

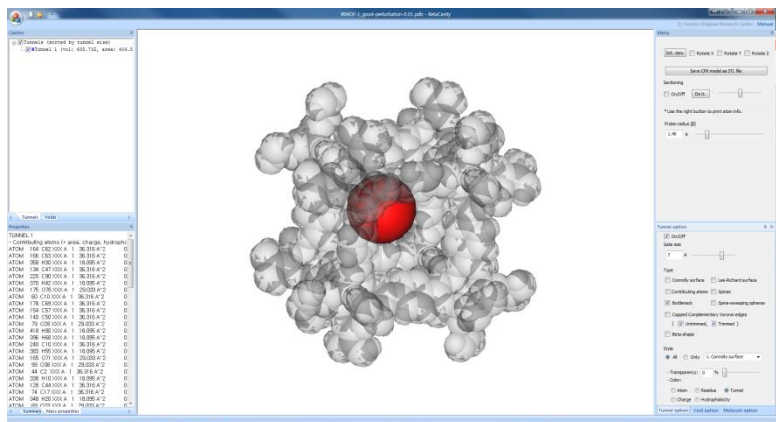
# Functions for Tunnels



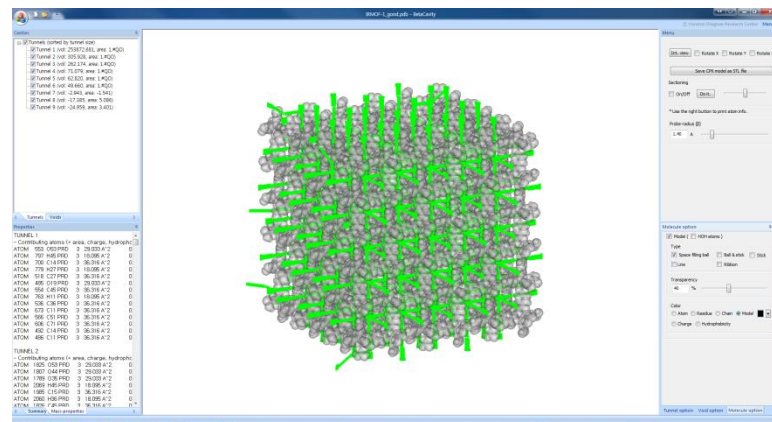
Calculating area / volume of a tunnel



Topology (spines) of a tunnel in MOF



Bottleneck of a tunnel



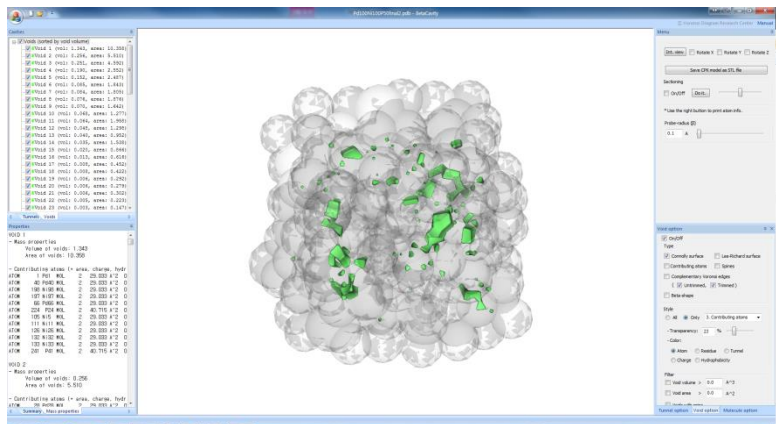
Tunnel in MOF (3x3 periodic structure)

# **Thank You**

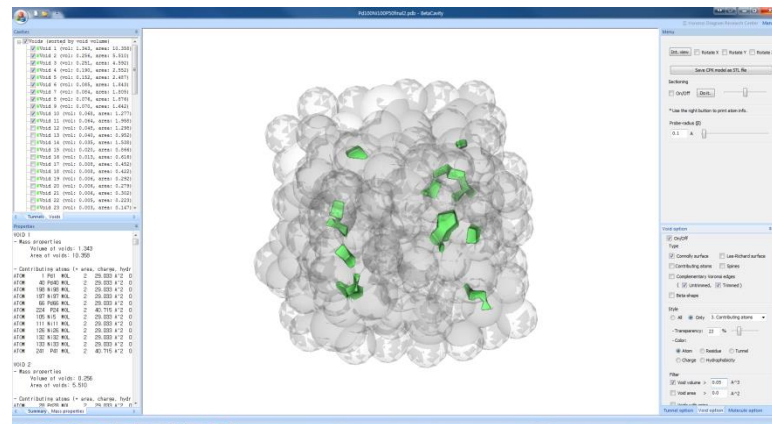
**- Welcome any collaborations -**

**<http://voronoi.hanyang.ac.kr>**

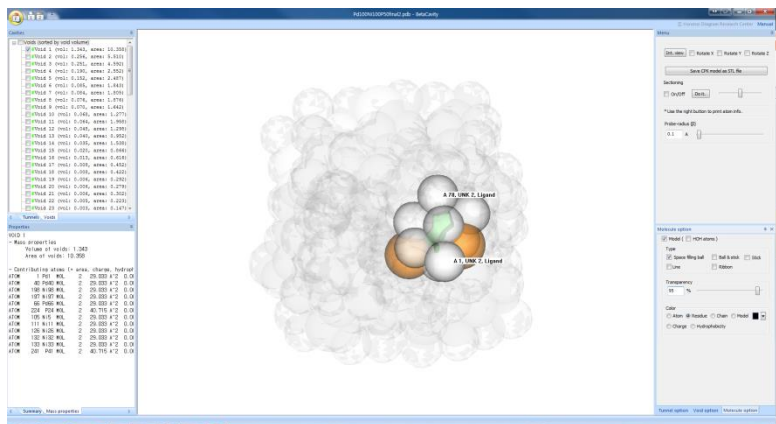
# Functions for Voids



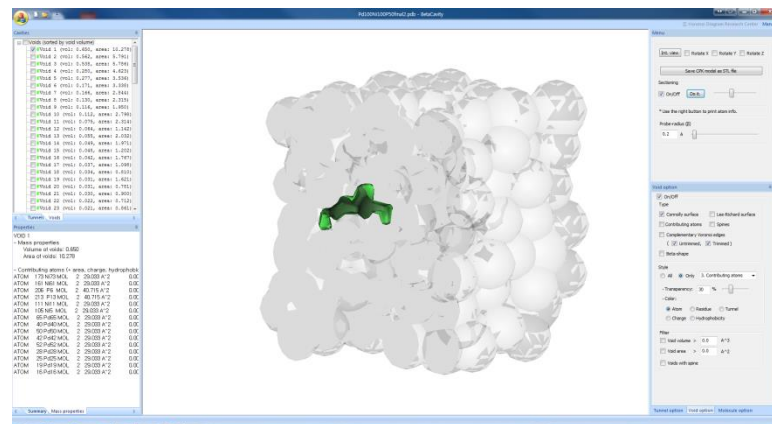
voids in amorphous material



Filtering by area / volume



Contributing atoms for biggest void



Sectioning to navigate inside of void