Calculation and Visualization of Molecular Surfaces

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In the presentation, I will introduce a new Voronoi-type diagram of balls, based on which different molecular surfaces can be completely characterized, especially the solvent excluded surface (SET). All surface singularities can be computed a priori and all inner cavities can be detected. In addition, molecular volumes and areas can be computed exactly.

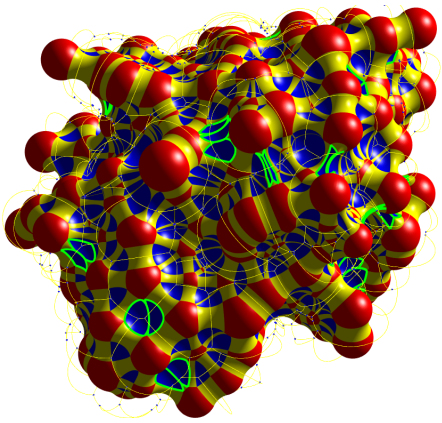

Figure 1: The SES of molecule 1B17. The green arcs are the boundaries of those SES-patches with singularities.

Joint work with: Benjamin STAMM.

References

[1] Chaoyu Quan, Benjamin Stamm. Mathematical analysis and calculation of molecular surfaces. *Journal of Computational Physics*, 322: 760-782, 2016.

[2] Chaoyu Quan, Benjamin Stamm. Meshing molecular surfaces based on analytical implicit representation. *Journal of Molecular Graphics and Modelling*, 71: 200-210, 2017.