

Algorithms of symmetry measurement

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The CSM (Continuous Symmetry Measure) was developed in the 1990s by Avnir, Peleg and Zabrodsky as a measure for the symmetry level of molecules ([1]).

For a given molecular structure, the calculation of the CSM is a nontrivial task. Over the past 8 years, we have developed exact and approximate algorithms for the calculation of the CSM in various conditions, depending on the size and type of the molecules ([2]-[5]).

It is natural to try to extend these methods to the symmetry analysis of crystals, where we could have a continuous scale on which the fit of a given crystal to a given space symmetry group will be measured.

In this talk I will focus on the algorithmic side of our work, and describe the methods we developed for molecules, and our work in progress towards extending them to the symmetry analysis of crystals.

Joint work with Inbal Tuvi-Arad.

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- [4] Gil Alon, Yuval Ben-Haim and Inbal Tuvi-Arad, Continuous symmetry and chirality measures: approximate algorithms for large molecular structures, *Journal of Cheminformatics*, 5, 106 (2023).
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