

## State-of-the-art and perspectives of implicit modeling for molecular surfaces

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### **Abstract:**

In this talk, we revise the theory of implicit surfaces and their applications to molecular surface modelling, such as blobby models and their variations. We will discuss their main properties, and their pros and cons with respect to alternative representations, such as the Euclidean distance transform and the skin surface. Then, we present recent applications of implicit modeling to (i) the local definition of molecular surfaces through constructive solid geometry, (ii) the identification of cavities for molecular simulation, and (iii) the representation of uncertainty in the computation of the molecular surfaces.