Improving Perception of Molecular Surface
Visualizations by Incorporating Translucency Effects

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Molecular surfaces are a commonly used representation in the analysis of molecular structures as they provide a compact description of the space occupied by a molecule and its accessibility. However, due to the high abstraction of the atomic data, fine grain features are hard to identify. Moreover, these representations involve a high degree of occlusions, which prevents the identification of internal features and potentially impacts shape perception. In this paper, we present a set of techniques which are inspired by the properties of translucent materials, that have been developed to improve the perception of molecular surfaces: First, we introduce an interactive algorithm to simulate subsurface scattering for molecular surfaces, in order to improve the thickness perception of the molecule. Second, we present a technique to visualize structures just beneath the surface, by still conveying relevant depth information. And lastly, we introduce reflections and refractions into our visualization that improve the shape perception of molecular surfaces. We evaluate the benefits of these methods through crowd-sourced user studies as well as the feedback from several domain experts.

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