Molecular surface

1 Introduction

It is well-known that the geometric structure of a protein is one of the most important factors which determine the functions of the protein. In particular, the smooth surface on the boundary atoms of a protein is one of the important geometric structures of the protein [3,2].

Suppose that a protein and a *spherical probe* are given (See Fig. 1(a)). The (spherical) probe represents a solvent molecule. Then, a smooth surface covering the boundary atoms of a protein can be defined by rolling a probe over the boundary atoms as shown in Fig. 1(b). This surface is called a *molecular surface* (**MS**) or *Connolly surface* after the researcher who first analytically defined the surface [2].

Indeed, a molecular surface is defined through the blending operation by a given probe. Hence, a molecular surface consists of two types of surfaces: (i) the surface of a boundary atom and (ii) the surface of a probe. The first one is called a (*solvent*) *contact surface* and the second one is called a *blending surface.*

If we see a **MS** in 3D (Fig. 1(c)), a blending surface is further categorized into two types: (i) the surface defined between two atoms (called a *rolling blending surface*) and (ii) the surface defined among three atoms (called a *link blending surface*). We call a individual small surface region of the surfaces a *patch*. Hence, **MS** consists of three types of patches: (i) a **contact patch** from a contact surface, (ii) a **rolling patch** from a rolling blending surface and (iii) a **link patch** from a link blending surface. Note that another **MS** with a different shape is defined if we change the size of a probe as shown in Fig. 1(d).

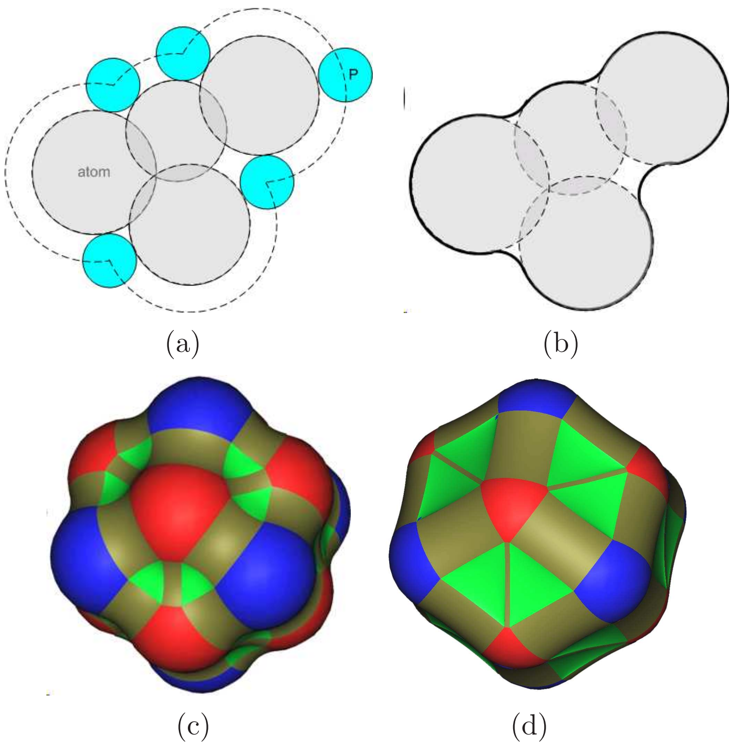


Fig. 1. Molecule and MS: (a) a molecule and spherical probe, (b) a molecular surface defined by a molecule and probe in (a), (c) a molecular surface in 3D and (d) a molecular surface corresponding to a larger probe than that of (c).

2 Three types of patches

2.1 Rolling patch

A rolling patch is defined while a probe rolls over two nearby atoms keeping in tangentially contact with the atoms. Hence, a rolling patch is a subset of the toroidal surface. Depending on the conditions, a rolling patch can be either complete or partial, and it may or may not self-intersect as shown in Fig. 2(a)-(d).

2.2 Link patch

A link patch is defined when a probe is on top of three nearby atoms. Then, the link patch is in principle triangular unless the link patch has no interactions with other link patches as shown in Fig 3(a). Therefore, the boundary curves of the link patch are completely determined by the sharing of the boundary with adjacent rolling patches. Note that this link patch has only three vertices and the adjacent rolling patches do not self-intersect.

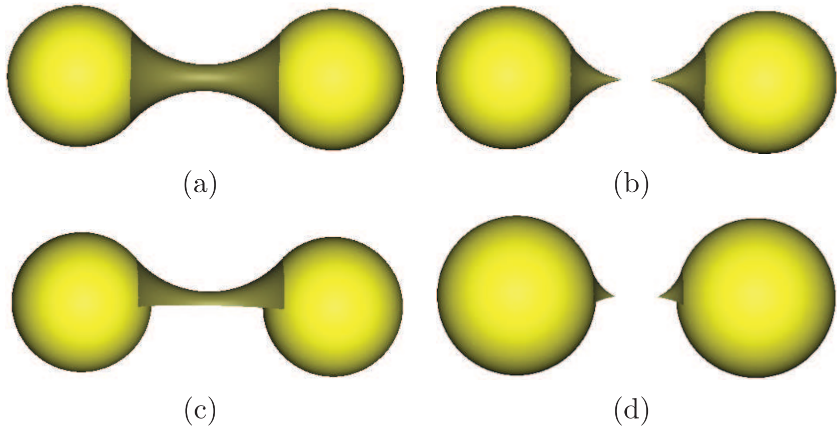


Fig. 2. Rolling patch: (a) complete non-self-intersecting rolling patch, (b) complete self-intersecting rolling patch, (c) partially revolved rolling patch, and (d) partially revolved self-intersecting rolling patch.

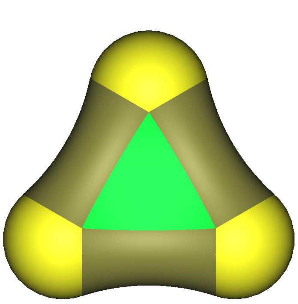
However, a link patch can have intersections with other link patches. There are two kinds of intersections among the link patches [1,4]. First, a link patch may intersect another link patch at the boundary. In this case, an in-between rolling patch necessarily self-intersects (See Fig. 3(b)). The link patch in the center of Fig. 3(b) intersects three other link patches and its topology is 9-sided.

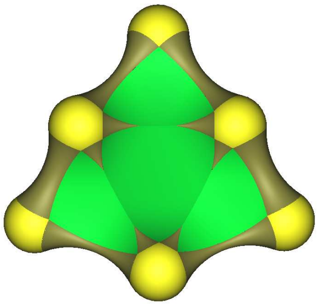
Second, a link patch may intersect another link patch to form a hole interior to itself (See Fig. 3(c)). A hole can be made by the intersection between two link patches which are located at the opposite sides of the associated atoms. It is also possible that both patches may have non-identical triplets of atoms for the hole.

While Fig. 3(b) shows the intersections by only adjacent neighbors, a link patch may also intersect other non-adjacent but neighbor link patches in $\mathbb{R}^3$. Fig. 3(d) and Fig. 4 show link patches trimmed by both adjacent and non-adjacent link patches. Note that the link patch in the center of Fig. 4 has three disconnected components by trimming of other link patches.

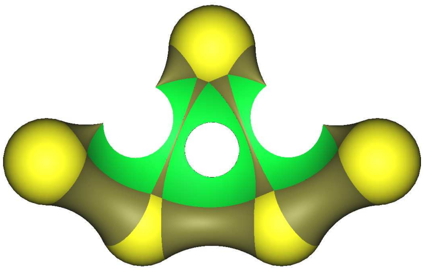
2.3 Contact patch

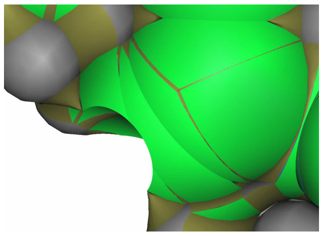
A contact patch is defined on the van der Waals surface of an boundary atom where a probe touches the atom. A contact patch is thus a spherical polygon on an atom bounded by a number of circular arcs and/or circles which are shared by adjacent rolling patches. Note that the boundary of a contact patch may be disconnected and may consist of more than one complete circle. Fig. 5(b) and (d) shows the contact patches of the atom in the center of Fig. 5(a) and (c). Note that each contact patch consists of two disconnected components.





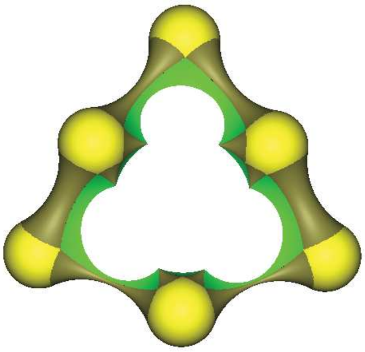
(a) (b)

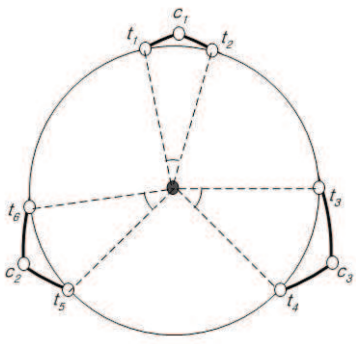




(c) (d)

Fig. 3. Link patch: (a) a link patch without intersections, (b) a link patch with intersections at the boundary, (c) link patches with intersections both at the boundary and in the interior, (d) a link patch with intersections by non-adjacent neighbors.





(a) (b)

Fig. 4. Trimmed link patch with disconnected components: (a) an example of trimmed link patch with disconnected components and (b) an illustration in 2D for (a)

References

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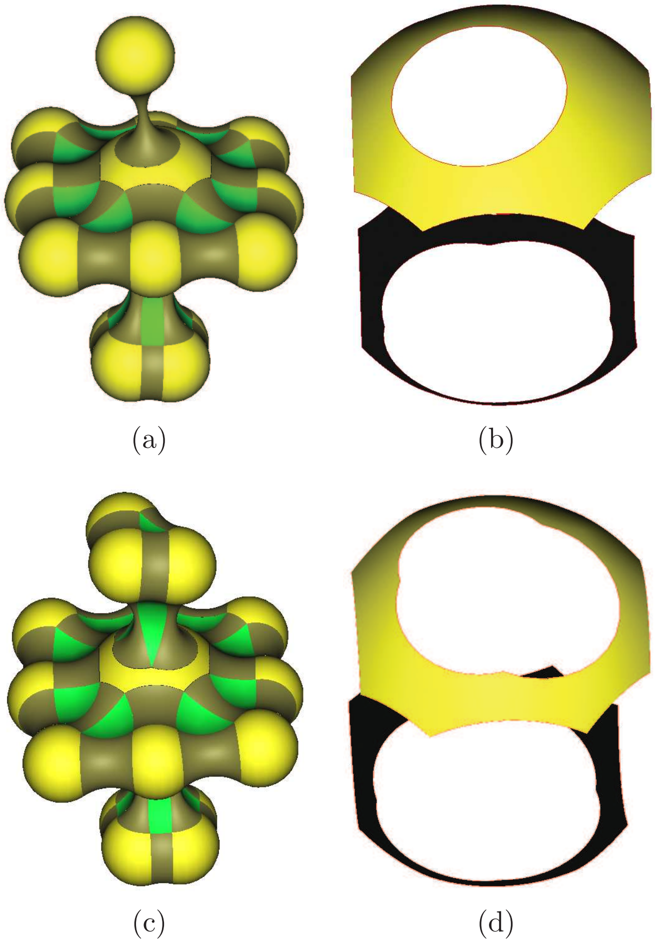

Fig. 5. Contact patches: (a) a molecule, (b) a contact patch of (a), (c) a molecule and (d) a contact patch of (c).

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