Molecular Visualization Principles for Science Animators

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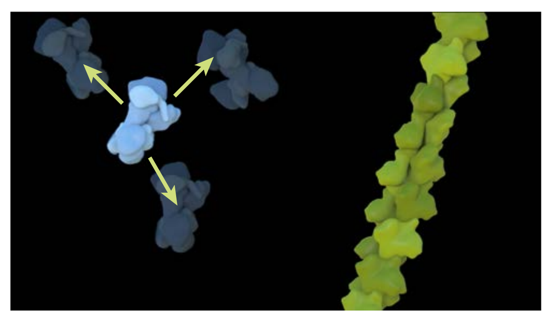
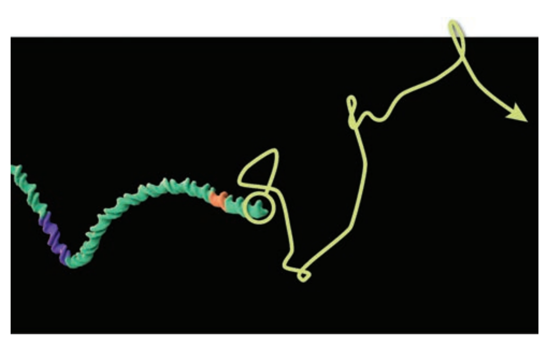
Misconceptions held by biology students grappling with an understanding of the molecular realm, typically relate to molecular processes (e.g. a cell signal cascade) and behaviours (e.g. Brownian motion). While dynamic visualizations may help to bridge this gap in understanding, frequently this is not the case. Either because of technical limitations, design constraints, or lack of awareness of fundamental concepts, animation may depict molecular environments with biophysically inaccurate properties, thus perpetuating misconceptions. Through our research examining visualization strategies, arose a series of animation design principles. We have identified 12 principles that serve as reminders of concepts and behaviours. Each principle is accompanied by a pair of short animations depicting both an example that does not adhere to the principle and one that does adhere to the principle. **These animations may be viewed at www.sciencevis.ca**



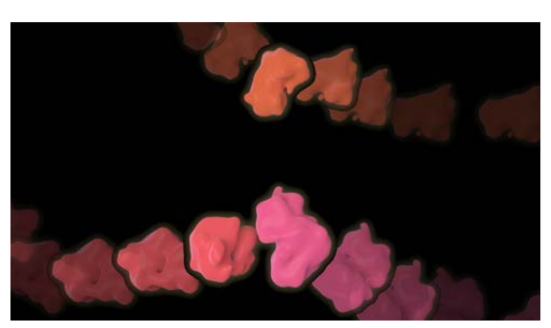
1 Molecules move through random collisions

Molecules move around through collisions resulting in random Brownian motion.



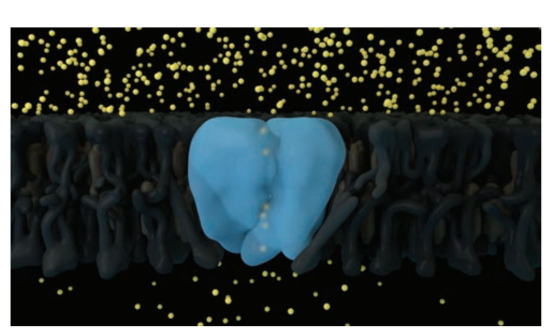
2 Long molecules experience similar forces along their length

The same forces are present along the full length of a long molecule. Putting a head to a molecule invokes agency.



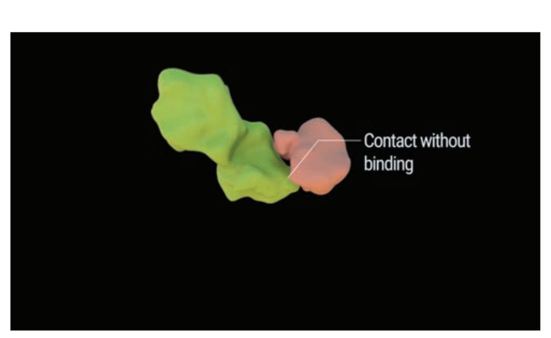
3 Molecules are in constant motion

Newton's first law states that objects remain in motion without external forces. While molecules are subjected to constant forces from all sides, the result is they are in constant motion and do not start and stop spontaneously.



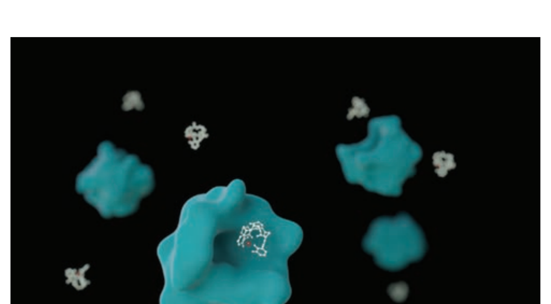
4 Intermolecular attractions are local forces

At this scale, showing negative pressure or distant molecules flooding toward a target invokes agency. The same applies to the relative motion between two binding partners.



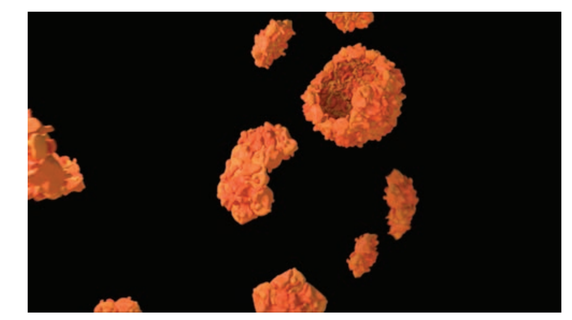
5 Unproductive collisions occur more often than productive ones

Not every encounter between complementary molecules results in binding; in fact statistically there are likely to be many more unproductive collisions than productive ones.



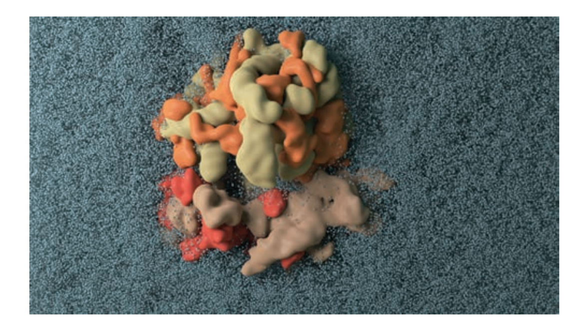
6 Many instances of molecules & events exist

There are typically many instances of molecules and events present in a given environment; repetition can also reinforce the process being depicted.



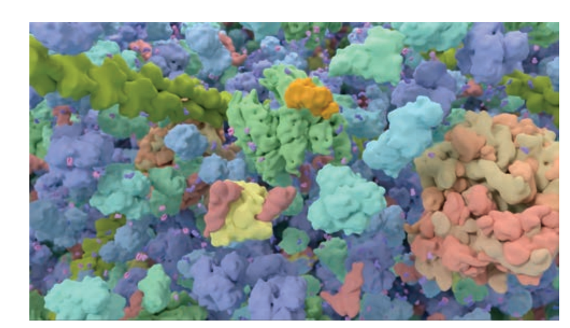
7 Not all instances of a molecule change state in a process

Not every molecule is used in a process or changes its state. More monomers are present than will be incorporated into a polymer, and typically more substrates are present than will be converted into a product.



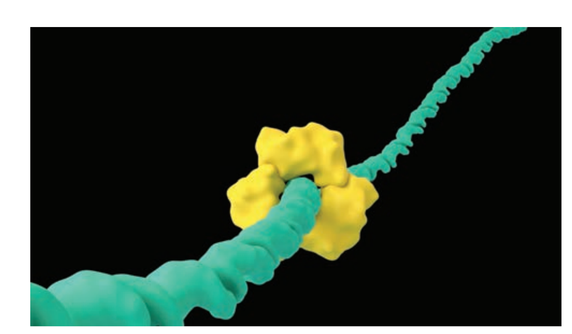
8 Light & molecular water do not produce macroscopic phenomena

Water is composed of molecules and light does not interact with it at that scale to produce macroscopic phenomena, like caustics, refraction, distortion, or crepuscular/god rays. These "underwater" effects are not relevant at the molecular scale.



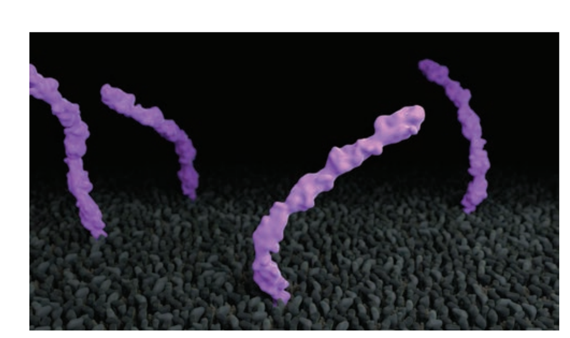
9 Molecular landscapes are crowded & diverse

Cellular environments are busy and crowded, with very little empty space, particularly if molecular water is included. Even without the depiction of molecular water, macromolecules take up a sizeable percentage of the volume.



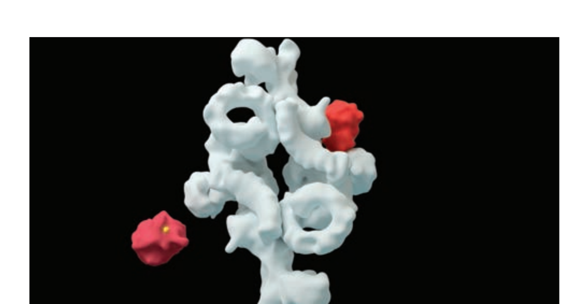
10 Molecules are physical entities with definable boundaries

Molecules are physical entities with definable boundaries. Intersecting surface meshes provide conflicting or obscured information about interaction and binding sites.



11 Proteins exhibit a range of flexibility

Proteins have internal freedom of motion that allows for specific functionality. Some parts of a protein are more flexible than others and some proteins are more rigid than others.



12 Many binding reactions are reversible before reactions occur

Molecules do not bind permanently and many reactions are reversible at the individual molecule level.