Scientists watch on the atomic level how individual molecules recognize each other

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The body is an almost perfect machine. For it to function properly, each individual component, that is each molecule, must reliably fulfill its specific function. Each molecule must thus “recognize” other molecules and work with them. A team of researchers from the Max Planck Institute for Solid State Research in Stuttgart, the Fraunhofer Institute in Freiburg, and King’s College in London, has now successfully filmed pairs of molecules during the recognition process. As reported to the journal *Angewandte Chemie*, the shapes of the molecules change to accommodate each other.

Like humans, molecules also “greet” each other with a kind of “handshake”. Anyone who has tried to shake someone’s right hand with his or her own left will have had a little trouble: the right and left hands do not fit together. In the same way, some molecules that exist in both a right-handed (D) and left-handed (L) configuration can tell if others they encounter are the D or L form.

Magali Lingenfelder and colleagues at the Max Planck Institute for Solid State Research have now been able to use scanning tunneling microscopy to take a series of pictures that follow in detail the “encounters” of diphenylalanine molecules adsorbed onto a substrate. (Diphenylalanine is the central structural unit within polypeptide fibers found in the brains of Alzheimer’s patients.) The “film sequences” reveal that only molecules with the same chirality (handedness) readily aggregate into pairs and chains.

Just as in a handshake, it is not enough that the right hands hold each other. To grip each other firmly, the two hands must adapt to fit their shapes together. Molecules do the same: close examination of the "film", in conjunction with theoretical calculations by researchers from King's College, prove that this type of dynamic accommodation of shape also occurs when two molecules "shake hands".

"Our work finally demonstrates that Linus Pauling was right with his theory of intermolecular conformation of over 50 years ago," says Lingenfelder. "In molecular recognition, it is not so much the static forms that are important, but rather how well the molecules can conform to each other."

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