Competing forces: How molecules maintain their structure

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A double helix twisted around itself: this is the distinctive structure of DNA, which is made up of large molecules. Using synthetically produced molecules, chemists and physicists at Martin Luther University Halle-Wittenberg (MLU) have investigated the forces which are at work inside the molecule to give it its three-dimensional structure. They have discovered that there are two primary forces at play that can strengthen or weaken one another. The scientists have recently presented their findings in the international edition of the journal *Angewandte Chemie*.

Two main parameters determine structure formation: hydrogen bonds that attract one another, and so-called phase segregation, which ensures that molecules repel each another. "It was previously assumed that the forces found in macromolecules had little influence over one another. There was a lack of research on forces contributing to structure formation, especially in solid polymers," says Professor Wolfgang H. Binder from the Institute of Chemistry at MLU. In order to better understand how the molecules interact, the researchers produced simplified polymers. They examined these polymers in close collaboration with a team of physicists from the University of Halle, led by Professor Thomas Thurn-Albrecht and Professor Kay Saalwächter.

Using x-rays and magnetic resonance spectroscopy, the scientists tested whether the molecules assembled or repelled each other. It was discovered that the forces on boundary surfaces have a particularly strong influence on each other. The degree of influence depends on the size of the molecule, increasing with its size. "The results help improve

our understanding of the structure formation of polymers," says Binder. They allow conclusions to be drawn about the material properties of, for example, self-healing materials, since the competing forces in such materials can now be more easily adjusted. Furthermore, the results enhance our knowledge about proteins, whose structures contribute significantly to their functionality.

More information: Senbin Chen et al, Opposing Phase-Segregation and Hydrogen-Bonding Forces in Supramolecular Polymers, *Angewandte Chemie International Edition* (2017). DOI: 10.1002/anie.201707363

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