Mark Hoffmann, Chester Fritz Distinguish Professor and computational chemist in the Department of Chemistry of the University of North Dakota has teamed with colleagues from the University of Oslo, Norway, to discover a new type of chemical bonding, distinct from the well-known covalent and ionic bonding.

Hoffmann and Tryve Helgaker, a well-known Norwegian scientist, and co-authors E.I. Tellgren and K. Lange have discovered a molecular-level interaction that science has puzzled over for decades but has never seen. In an article published recently in the internationally respected journal Science, A Paramagnetic Bonding Mechanism for Diatomics in Strong Magnetic Fields, Science 20 July 2012: Vol. 337 no. 6092 pp. 327-331. DOI: 10.1126/science.1219703, Hoffmann and his colleagues describe their use of quantum chemical simulations to model the bonding in diatomic hydrogen and also diatomic helium in extreme magnetic fields – extremes that are only attainable (at present) in stars near the end of their life.

Ordinary covalent or ionic bonds would fall apart under these conditions. However, within magnetic fields approaching half a million Tesla (versus the thousandth of one Tesla of a fridge magnet), the research team has shown that a net attraction could develop between two adjacent atoms when their spin states align. They have called this interaction ‘perpendicular paramagnetic bonding’ and have made predictions about the light emissions of these oddly bonded species. Perpendicular paramagnetic bonding is the stabilization of the anti-bonding $\sigma_u$ orbital in the presence of a magnetic field. This stabilization occurs because a magnetic field lowers the energy of orbitals that correspond to counter-clockwise rotation. Normally, one would not think of an anti-bonding $\sigma_u$ orbital as having the favored rotation (angular momentum), but a detailed analysis shows that it in fact it does in the presence of a magnetic field, provided that the orientation of the molecule is perpendicular to the field.

It is now up to astronomers and astrophysicists to see if the spectral signatures of these species can be detected in the emissions of white dwarf and other aged stars. "We computationally modeled [a bonding] behavior that we theorized, based on universally applicable physical principles," said Hoffmann, an internationally recognized expert in the theory and computational methods used for elucidating molecular electronic structure. "We discovered a new type of chemical bonding. That's a pretty bold statement, but I'm not kidding you! It's a brand new type of chemical bonding, not previously known to science." "Our discovery addresses one of the mysteries in astrophysics about the spectrum of white dwarf stars," Hoffmann said. "White dwarfs have an unusual spectrum that has been thought to result from polymerized hydrogen and helium, which of course do not occur on Earth."

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