Chirality-induced spin polarization places symmetry constraints on biomolecular interactions

The work examines the fundamental relationship between an electron's spin and a molecule's chiral symmetry. The spin of an electron is a pure quantum mechanical property and specifies its intrinsic angular momentum. A common classical analogy for the electron spin is to describe it in terms of a child's toy, a spinning top. Like a spinning top which can rotate clockwise or counterclockwise, an electron has two spin states, referred to as "spin-up" and "spin down". Chiral molecules are the building blocks of life. Chirality is the name for a symmetry and originates from the Greek word 'cheir', for hand. Indeed, the human hand displays chiral symmetry; namely an individual hand has no mirror symmetry but a mirror symmetry exists between our right and left hands. In more precise language, our two hands are called enantiomers of one another. Similarly, chiral molecules are referred to as being a right-handed enantiomer or a left-handed enantiomer.

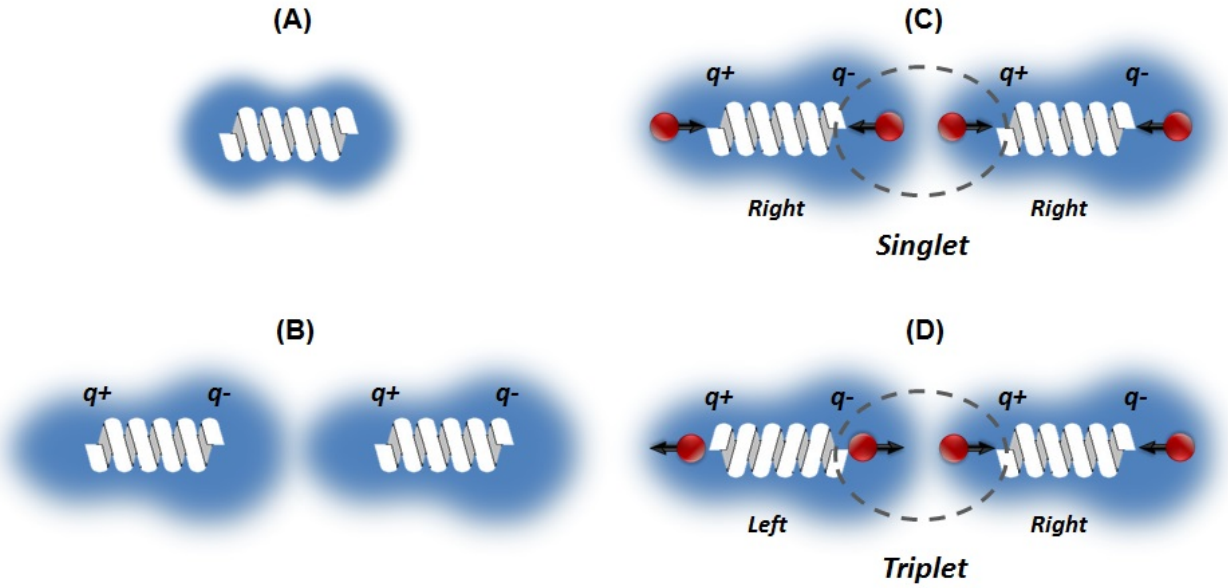

Fig. 1. A) The schematic diagram illustrates the electron distribution (blue cloud) in a molecule that does not have a dipole moment, before it interacts with another molecule. In this case the distribution is symmetric. B) This diagram illustrates the electron distribution when two molecules interact via dispersive forces. The interaction induces an asymmetry in the electrons' distribution resulting in an "induced dipole" in each molecule. This charge polarization causes an "induced-dipole induced-dipole" interaction. C) The diagram illustrates the induced dipole interaction of two molecules with the same handedness. As charge q transfers from one side of the molecule to the other, it generates a spin polarization (represented by a red ball and black arrow) of the same spin in the two molecules. The electron density left behind has therefore the opposite spin polarization, hence the interaction between the molecules is characterized by two opposite spins, as illustrated by the dotted circle-singlet region. D) When the two interacting molecules are of opposite chirality

the interaction between the molecules is characterized by two spins parallel to each other (in the dotted circle-triplet region).

While it is difficult to separate two different enantiomers of the same molecules artificially, in Nature this process is efficient. The present work proposes a new mechanism for understanding this efficiency. It is based on former works that established that the efficiency of electron motion through chiral molecules depends on their spin. In many bio-processes, the interactions between molecules result from electron reorganization in the molecules, like that which occurs when an external electric field is applied. We show that the charge reorganization in chiral molecules is accompanied by a polarization of the spins associated with the displaced charge. The symmetry constraints imposed by this spin polarization may account for the enantioselectivity. Calculations indicate that this contribution to the interaction energy for two molecules of the same handedness can be comparable to the thermal energy.

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