Strong chirality-induced spin polarization in twisted transition metal dichalcogenides

Guido Menichetti[a]
Lorenzo Cavicchi[b]
Leonardo Lucchesi[a,c]
Fabio Taddei[d,b]
Giuseppe Iannaccone[c]
Pablo Jarillo-Herrero[e]
Claudia Felser[f]
Frank H. L. Koppens[g,h]
Marco Polini[a,g]
[a] *Dipartimento di Fisica dell'Università di Pisa, Largo Bruno Pontecorvo 3, I-56127 Pisa, Italy*
[b] *Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa,Italy*
[c] *Dipartimento di Ingegneria dell'Informazione dell'Università di Pisa, Via Girolamo Caruso 16, I-56122 Pisa, Italy*
[d] *NEST, Istituto Nanoscienze-CNR, Piazza S. Silvestro 12, I-56126 Pisa, Italy*
[e] *Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA*
f Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, Dresden 01187, Germany
[g] *ICFO-Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, Av. Carl Friedrich Gauss 3, 08860 Castelldefels (Barcelona), Spain*
[h] *ICREA-Instituciò Catalana de Recerca i Estudis Avançats, Passeig de Lluìs Companys 23, 08010 Barcelona,Spain*
guido.menichetti@df.unipi.it

Abstract

In 1999, under the leadership of R. Naaman, a team made a significant observation: films composed of chiral organic molecules exhibit an asymmetrical scattering of polarized electrons [1]. This phenomenon, now widely known as the chirality-induced spin selectivity (CISS) effect, has garnered considerable attention in the field of chiral chemistry, yet much of its intricacies remain to be fully grasped [2]. Essentially, the CISS effect entails electrons passing through chiral molecules gaining a notable degree of spin polarization. In this study, we delve into the behavior of atomically-thin chiral crystals formed by twisting van der Waals heterostructures. In this work, we demonstrate that even in systems comprising just two monolayers, particularly those with spin-orbit coupling, this effect can be remarkably pronounced. Its emergence is attributed to the interplay between structural chirality and spin-flipping spin-orbit coupling. Through calculations involving twisted homobilayer transition metal dichalcogenides [3-6], we illustrate that the chirality-induced spin polarization can reach staggering proportions, exceeding 50% for materials like $MoTe_2$. Additionally, we introduce a theoretical framework for this phenomenon based on the microscopic Hamiltonian of twisted homobilayer transition metal dichalcogenides and a spin-resolved scattering matrix approach [7,8]. Our findings suggest that twisted quantum materials offer a versatile platform for investigating and manipulating the CISS effect in both condensed matter physics and chiral chemistry [9].

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