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Electric field control of donor pair *diatomic molecules* in silicon ALEJANDRA BAENA, Instituto de Física-Universidade Federal do Rio de Janeiro, ANDRE SARAIVA, Uniersity of Wisconsin-Madison and Instituto de Física-Universidade Federal do Rio de Janeiro, MARÍA J. CALDERÓN, Instituto de Ciencias de Materiales de Madrid ICMM-CSIC, BELITA KOILLER, Instituto de Física-Universidade Federal do Rio de Janeiro — Single donors are well-established building blocks for engineering electronic properties of semiconductors, acting effectively as giant hydrogen atoms [1]. Donor pairs, analogous to effective hydrogen molecules, were recently investigated [2,3] in the strongly interacting regime in silicon. In this regime, electric field control renders timid results. Pairs that are more distant are more susceptible to external fields, and may harbour single electron charge control. Theoretically, the molecular quantum mechanics analogy between a donor pair and the H_2 molecule in vacuum is not as straightforward as it may seem. A detailed understanding of the electronic structure of these molecular systems is a current challenge. We analyze the lowest energy states within effective mass theory, including central cell corrected donor potential effects and the conduction band multiplicity in Si. The spectrum of ionized donor pairs and its response to an external electric field will be presented. We contemplate possible advantages of heteropolar diatomic molecules, e.g, Sb−As pairs, as more efficient elements for such devices and applications.

[1] Zwanenburg et al., RMP,85,961 (2013).
[2] M. F. Gonzalez-Zalba et al., Nano. Lett.14,5672 (2014).
[3] Dehollain et al., PRL,112,236801 (2014).

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