The effect of a vibrational mode on the electronic properties of a deformable spin-1 molecule, in a break junction setup.

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structure-based design of novel inhibitors using virtual screening approaches. fCatB inhibitors abrogate the parasite life cycle and have a low selectivity regarding the specific host proteases, human (hCatB) and bovine (bCatB) cathepsins B. The Maybrigde Hit-finder is a 14,400 compound cluster base library based on the Lipinski´s rule of five and gives a selection of drug-like compounds, and once a hit is found, it gives about 10 closely related compounds that can be screened for a follow up prior to any synthetic procedure. In this work, we predict five putative selective inhibitors of fCatB by combining comparative modeling (multiple structures complex template), molecular docking (CA074, a dipeptidyl nitrile and Maybrigde Hit-finder compounds) and molecular dynamic simulations. The cathepsin B complex systems were stable after 50ns according to the RMSD. Cavitie´s prediction, ligand interactions and molecular dynamic simulations were made. Also, 13 potentially determinant residues for the substrate specificity were identified, and it was suggested that tree of them could enhance the design of selective cathepsin B Fasciola hepatica inhibitors regarding to mammalian cathepsins.

[1] Law, R.H., Smooker, P.M., Irving, J.A., Piedra, D. E., et al (2003) Infect. Immun. 71(12): 6921-6932.
[2] Zhou, Z., Wang, Y. & Bryant, S.H. (2010) J Mol Graph Model. 28(8): 714-727.

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Poster #12
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Title/Abstract: Using numerical renormalization group calculations, we study the effect of a vibrational mode on the electronic properties of a deformable spin-1 molecule, in a break junction setup. Stretching the molecule along the transport axis introduces a static magnetic anisotropy, as shown by experiments[1]. Our results indicate that a spin-vibron coupling can also contribute to the net anisotropy, countering the effects of stretching and driving the system through a quantum phase transition into a non-Fermi-liquid ground state, going through a Kondo quantum critical point with enhanced zero-bias conductance through the device.

[1] Science 328 1370 (2010)
[2] Phys. Rev. B 86, 035437 (2012)