Abstract Submitted
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QMC study of molecules for spintronics and photoswitching[1] MATUS DUBECKY, RENE DERIAN, LUCIA HORVATHOVA, Inst. of Physics, Slovak Academy of Sciences, Bratislava, Slovakia, LUBOS MITAS, Dept. of Physics, North Carolina State University, Raleigh, 27695, U.S.A., IVAN STICH, Inst. of Physics, Slovak Academy of Sciences, Bratislava, Slovakia — A combination of QMC and quantum chemistry (CAS-SCF) techniques are used to study two large molecules: azobenzene (AB) imporatnt as a photoswitch and vanadbenzene (VB), frequently used in spintronics [1]. In AB higher singlet state, S_2 the fingerprint of AB in excitation spectra has been calculated in addition to the low singlet states S and S_1 [2]. We have also calculated the lowest triplet T_1 vertical excitation, identified by EELS [3] as well as adiabatic T_1 excited state. All calculated energies are in excellent agreement with available experiments [3, 4]. In VB we focus initially on PES for dissociation and excited state of the vanadium cation.

[1] V.V. Maslyuk et al., Phys.Rev.Lett. 97, 201, (2006). [2] M. Dubecky et al., J.Chem.Phys, accepted (2010). [3] M. Allan, private communication. [4] J.-Å. Andersson, R. Petterson, L. Tegnér, J. Photochem. **20**, 17 (1982).

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