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Azobenzene optical switch controlled by external force[1] MARTIN KONOPKA, Slovak University of Technology, NIKOS DOLTSINIS, DOMINIK MARX, Ruhr-Universitaet Bochum, IVAN STICH, Slovak University of Technology
— External pulling force can be employed to manipulate optical switching properties of azobenzene molecule which is a promising system for molecular electronics devices. We perform density functional treatment of azobenzene terminated by S-H groups with pulling force applied via restraints on the sulfur atoms. We treat the system both at zero and room temperature and among other quantities focus on separation between ground (S0) and first excited (S1) singlet states. The separation is crucial for cis $\leftrightarrow$ trans reisomerization rate. For trans isomer we observe decrease of the S1-S0 separation with increased stretching force and the molecule length. For cis isomer we find opposite: the separation increases thus lowering photoisomerization rate. Another interesting point is mechanically induced cis $\rightarrow$ trans inversion in the ground state which occurs for extensions above 5 Å.

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