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Mechanically induced cis to trans reisomerization of azobenzene¹ ROBERT TURANSKY, MARTIN KONOPKA, IVAN STICH, Slovak University of Technology, DOMINIK MARX, Ruhr Universitaet Bochum — Using density functional techniques we study mechanochemistry of the azobenzene molecule. Azobenzene is an optically switchable molecule. Laser light is normally used to achieve molecular switching between the cis and trans isomers. We use mechanochemistry to achieve the switching. Thiolate-gold bond can used to exert mechanical energy on the molecule bonded between two gold electrodes in static AFM apparatus. Our model consists of two realistic gold electrodes bridged by dithioazobenzene. We find that pulling the transisomer leads just to formation of gold nanowires and mechanical breakage of the electrodes. However, mechanochemistry with modest applied forces leads to $cis \leftrightarrow trans$ reisomerization via rotation mechanism. Contrary, use of simple constraints instead of realistic gold electrodes, leads to $cis \leftrightarrow trans$ reisomerization, albeit with significantly larger applied forces and via inversion mechanism. Important experimental and theoretical ramifications of these simulations will be discussed.

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