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## Theoretical investigations on carbonyl sulfide (COS) and C<sub>60</sub>: Is C<sub>60</sub> a perfect Faraday cage? A possible nano storage device

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In order to operate a binary storage unit some basic requirements have to be satisfied. The unit needs to have two distinct, steady states that are erasable, programmable, detectable and insensitive against environmental influences. We therefore theoretically investigated fullerene complexes, which incorporate polar molecules. The complexes were orientated as monolayers on different metal surfaces (Au, Al, Ag). In preliminary calculations the binding energies and structural properties of CO and C<sub>60</sub> were calculated using the VASP code. The results showed that the orientation of CO towards the surface has no influence on the energies i.e., the molecule rotates freely inside the cage as known from literature for isolated CO and C<sub>60</sub>. In the following the carbon monoxide was replaced by the larger carbonylsulfide (OCS). The calculations then showed different energies with the oxygen atom or the sulfur atom facing towards the surface. These two states are separated by a rotation barrier of about 0.05 eV. Simulated STM-images showed that both states are detectable and distinguishable from outside the cage. The process of programming the storage device contains an alignment of the OCS molecules. A conceivable procedure of a successful orientation of the polar molecules inside the fulleren is the application of external electric fields. We therefore currently examine the shielding of the C<sub>60</sub> molecule in terms of the properties of a perfect Faraday cage.

### Biography

Oliver Potzel has completed his PhD at the age of 39 years from the University of Ulm and Postdoctoral studies from the Institute of Theoretical Chemistry.

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## Tribology of Al base nanocomposite reinforced with CMA nanoparticles after extrusion

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The present work focuses on studies of manufacturing and investigation of hardness and tribological behavior of aluminum alloy matrix composites (AAMCs) reinforced with various volume fractions of particles made of complex metallic alloys (CMAs). Microstructure refining after extrusion helped reduction of friction coefficient and wear rate in higher normal loads at room and elevated temperature. Scanning electron microscopic observation of the worn surfaces was conducted and the dominant wear mechanism was recognized to be abrasive wear accompanied by some delamination wear. X-ray diffraction and transmission electron microscopy (TEM) tests were carried out to investigate the formation of single phase nanoparticle of after several hours of milling.

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