

## The healing mechanism for excited molecules near metallic surfaces

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Examining individual molecules at the atomic scale is one of the most challenging problems of modern science. When crystallization of a molecule is difficult or impossible, an X-ray, electron, or positron micro-beam can act as a probe that enables the scientist to determine the structure of a single molecule. However, the beam itself can damage the molecule, in which case the molecule becomes fragmented before its structure can be determined.

This paper suggests, for the first time, a technique involving adsorption of the molecule on a weakly interacting metallic surface to reduce or compensate the radiation damage - the so-called "healing" mechanism (see Fig.1). The idea is that coupling the molecule with a (noble)-metal surface causes electronic excitations to dissipate within the characteristic time-scale of molecular vibrations. Excitations due to the incident beam are neutralized by charge transfer from the substrate, and subsequent Auger de-excitation, in a time interval that is shorter than the fragmentation time.

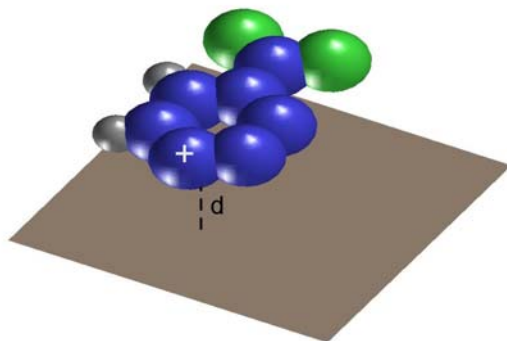


Figure 1. Schematic of a typical healing mechanism set-up: an ionized molecule is placed above a metallic substrate and the positive charge is at a distance  $d$  from the substrate. In this example, atoms of a PTCDA molecular fragment are shown. The small grey spheres denote H, the large green spheres denote O and the blue large spheres denote C.

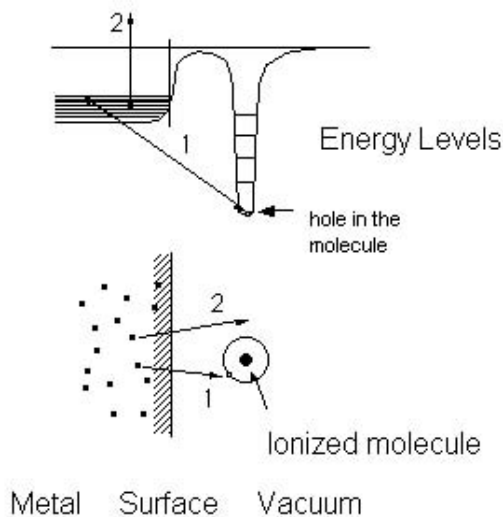


Figure 2. Schematic of the Auger Neutralization: As a first step a conduction electron (1) tunnels from the metal to neutralize the ion. Energy is released by electron (1), and this energy is transferred to a conduction electron (2) in the metal (figure adapted from Jan Axelsson's Doctoral dissertation at Uppsala University 1995).

The physics of the healing mechanism is closely related to the Auger Neutralization, shown in Fig. 2, which has been studied for decades in various fields. However, most of the previous work describes collisions of slow ions with solids, while the present study involves the neutralization of electronic excited physisorbed molecules on metallic surfaces. Given the wide range of estimates of the neutralization time in the literature, we provide a conservative estimate to demonstrate the feasibility of the healing mechanism in the present case.

A recent method using interference patterns with standing x-ray waves has been used to map the perylene-tetracarboxylic-dianhydride (PTCDA) molecule on a silver surface (see A. Hauschild et al., Phys. Rev. Lett. 94, 036106 (2005) see also Physics News Update, Number 717 (Story #2), 2005). The feasibility of this new experiment and other earlier experiments involving PTCDA molecules on metallic surfaces (see e.g. Y. Hirose et al., Phys. Rev. B 54, 13748 (1996)) suggest that the "healing mechanism" near a metallic surface works well.

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