

A post-doctoral position is immediately available in the GNS group of CEMES (CNRS lab Toulouse) in close collaboration with the MPC group (Physical and Chemical Modeling) of LPCNO laboratory at the INSA-Toulouse, both located in Toulouse, France. The position, funded by a NanoX collaborative initiative, is for one year. The net salary should be around 2200 and 3200 \in depending on the working experience.

The STEFE project aims at studying, mainly theoretically, the local electric field inside a scanning-tunneling-microscope junction. This EF is usually generated by a bias voltage applied between the local probe and the metallic substrate. Due to the tip shape, a more or less strong enhancement of the EF exists beneath the apex and can modify the adsorption state of a single atom or a single molecule according to the bias voltage and the tip-surface distance. Without an atomic-scale description of the tip apex and its effects on the adsorbates, the EF effect remains unclear. We plan to rationalize the possible EF enhancement in various situations with the help of DFT calculations, as well as a N-body order method. We shall apply our numerical methodology to molecular adsorbates with an increasing complexity, starting with single atoms to complexe molecules dedicated to the NanoCar Race 2021 (NCR21).

The ideal candidate, willing to collaborate in an interdisciplinary team in connection with experimentalists, is required to have a Ph.D in materials science or quantum chemistry as well as a strong background and an extensive working experience in first principles electronic structure calculations. Basic knowledge on STM techniques are expected also.

For further information on the CEMES and LPCNO involved research groups please visit the websites <u>http://www.cemes.fr</u>, <u>http://www.lpcno.insa-toulouse.fr</u>. A completed applications should include a CV, a cover letter and three contact references to Dr. X. Bouju **and** to Dr. I. Gerber by e-mail (<u>bouju@cemes.fr</u>, <u>igerber@insa-toulouse.fr</u>). Screening of the applicants starts now and will continue until the position is filled. More information can be found here: <u>https://bit.ly/37li8sT</u>.