

Realizing a dream in nanoscience: simultaneous measurement of the local atomic and electronic structure of a crystalline material.

Auke Vlasblom, Victor Wesselingh, Ingmar Swart, [Daniel Vanmaekelbergh](#)

Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, Univ. of Utrecht

Connecting the (local) atomic structure of a crystal to its electronic band structure would be of great value in solid state- and material science, including photovoltaics. In the field of nanocrystals, attempts have been made to measure the optical response of an individual nanocrystal and measure afterwards the shape and crystal structure of the same nanocrystal with TEM or STEM (1). However, the optical response is only indirectly connected to the band structure, while transmission electron microscopy provides the shape of the crystal and the atomic columns in the beam direction, but it is generally difficult to image the point defects. We claim that scanning tunneling microscopy and spectroscopy is one of the few techniques that can give a reasonably complete picture of the local electronic and atomic structure by simultaneous measurement of the atomic topography and the density of states. However, the synthesis of a crystal of interest in a UHV chamber or the transfer of a crystal from outside into an ultra-clean STM environment is very cumbersome and limits this method to dedicated research groups.

We present a method to transfer wet-chemically prepared nanocrystals into ultra-high vacuum on an ultra-clean metallic substrate surface by a new stamp method; this allows one to obtain atomic resolved images of the nanocrystal and the substrate surface. In the case of two-dimensional Bi_2Se_3 (nanoplatelets), which we investigate for their electronic topology and unusual optical properties, we were able to resolve the atomic structure and all surface and sub-surface point defects. From the dI/dV density of states we obtain the overall band structure of the unperturbed crystal and around defects. We distinguish point defects that do not affect the band structure at all, such as the Se-vacancy that acts as a dopant from point defects that feature an extra electronic resonance. The latter are expected to be active in the trapping and recombination of photogenerated carriers.

1. ***Correlation of atomic structure and photoluminescence of the same quantum dot: Pinpointing surface and internal defects that inhibit photoluminescence.*** Orfield, N. J., McBride, J. R., Keene, J. D., Davis, L. M. & Rosenthal, S. J., *ACS Nano* **9**, 831–839 (2015).

2. Auke Vlasblom, Victor Wesselingh, Ingmar Swart, Daniel Vanmaekelbergh, submitted

3. ***Scanning probe microscopy and spectroscopy of colloidal semiconductor nanocrystals and assembled structures*** Swart, I., Liljeroth, P. & Vanmaekelbergh, D.. *Chem Rev* **116**, 11181–11219 (2016)

4. ***Characterization of the Edge States in Colloidal Bi_2Se_3 Platelets.*** Moes, J. R. *et al.*. *Nano Lett* **24**, 5110–5116 (2024)

5. ***Role of Surface Bands in the Photogeneration, Cooling, and Recombination of Charge Carriers in Two-Dimensional Bi_2Se_3 .*** J. F. Vliem *et al.*, *ACS Nano* 2025, 19, 18, 17261–17272