

Role of INS Spectroscopy And DFT Calculation For Investigating the C-H Terminations In Activated Carbons

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Activated carbons have a great importance in several sectors, ranging from adsorbent materials to heterogeneous catalysis. In the last years our group studied several activated carbons characterized by different activation and post-activation procedures employed as catalysts' supports. All these samples have been provided by Chimet S.p.A, in the frame of a long-lasting collaboration. Among the characterization techniques employed, INS spectroscopy has demonstrated to be a very powerful technique, being particularly sensible to the C-H terminations at the edges of the graphitic domains. The measurements were performed on the TOSCA instrument at ISIS^{1,2} and on LAGRANGE at ILL³, and further measures are planned in the near future.

The assignment of the bands observed in the experimental spectra to specific vibrational modes is a challenging task. The simulation of INS spectra by means of DFT calculations has the potential to shade new light on several details otherwise impossible to determinate⁴. In the frame of our simulation work, we demonstrated that the main features of the experimental spectra can be well simulated by using simple models consisting in polycyclic aromatic compounds (Figure 1a). Furthermore, simulations also allowed us to discriminate the contribution of C-H occupying different positions along the borders, thus allowing us to assign specific peaks in the experimental spectra to specific border geometries (Figure 1b). By simulating the spectra of a large number of different models it was possible to understand the contributions to the spectra of several border geometries, determining which one displays the best agreement with the experimental spectra and thus which kind of C-H termination geometries are more likely to be present within our samples.

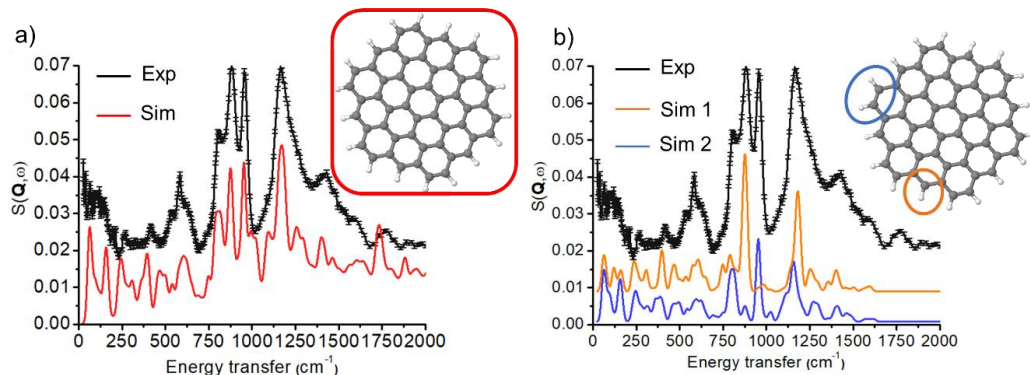


Figure 1: part a) Comparison between the experimental spectrum of a physically activated carbon compared with the simulated spectrum of one of the models considered in this study. Part b) comparison of the same experimental spectrum with the simulated spectra of the single contributions of two different C-H border sites.

1. A. Lazzarini; A. Piovano; R. Pellegrini; G. Leofanti; G. Agostini; S. Rudić; M. R. Chierotti; R. Gobetto; A. Battiato; G. Spoto; A. Zecchina; C. Lamberti E. Groppo, *Catal. Sci. Technol.*, **2016**, 6, 4910-4922
2. A. Lazzarini; R. Pellegrini; A. Piovano; S. Rudić; C. Castan-Guerrero; P. Torelli; M. R. Chierotti; R. Gobetto; C. Lamberti; E. Groppo, *Catal. Sci. Technol.* **2017**, 7, 4162-4172
3. M. Carosso; A. Lazzarini; A. Piovano; R. Pellegrini; S. Morandi; M. Manzoli; J. G. Vitillo; M. Jimenez-Ruiz; C. Lamberti; E. Groppo, *Faraday Discuss.* **2018**, Accepted Manuscript DOI: 10.1039/C7FD00214A
4. A. Piovano; A. Lazzarini; R. Pellegrini; G. Leofanti; G. Agostini; S. Rudić; A. L. Bugaev; C. Lamberti; E. Groppo, *Advances in Condensed Matter Physics*, **2015**, 2015, Article ID 803267