UNIVERSITÀ DEGLI STUDI DI MILANO

# SEMINARI ERC

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SEMICOMPLEX

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| Data | ***Venerdì 13 Aprile 2018, ore 11:00***<br>***Aula Montanari, Dipartimento di Chimica*** |
| Oratore | **Prof. Matteo Tommasini**,<br>Dipartimento di Chimica, Materiali e Ingegneria Chimica Giulio Natta, Politecnico di Milano |
| Titolo | **Vibrational fingerprints of molecular structure: the case of Polycyclic Aromatic Hydrocarbons** |
| Coordinatore | **Michele Ceotto**<br>*Dipartimento di Chimica* |

**Abstract**: Thanks to the developments in computer hardware and quantum chemistry we face exciting scenarios in theoretical vibrational spectroscopy. On the one side, increasingly large molecular systems can be addressed by DFT methods so that experimental vibrational spectra can be interpreted on the light of unprecedented theoretical data, enriching the existing empirical understanding of the vibrational spectra of big molecules. On the other side, vast vibrational structure datasets can be computed in a relatively short time, thus opening new possibilities for approaching difficult conformational problems, or the analysis of samples with a complex molecular structure. Tools from Statistics are thus very valuable for the efficient screening and rapid understanding of datasets composed by hundreds of entities, which would be otherwise very difficult to sort out by human inspection, on a one-by-one basis.

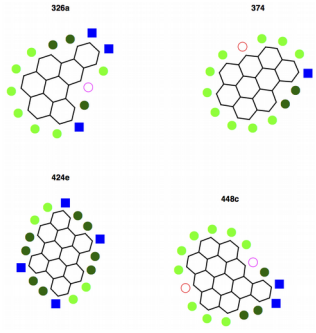


Fig.1 Structures of some of the PAHs considered, with different CH bonds.

The vibrational structure of fifty-one Polycyclic Aromatic Hydrocarbons (Fig. 1) has been analyzed in order to find spectroscopic signatures useful for the molecular characterization of complex samples of combustion origin [1]. The outcome of this analysis, carried out with statistical tools, is the identification of spectroscopic markers in the IR that carry significant information about the topology of CH bonds at the molecular edge. These results show the usefulness of IR spectroscopy for characterizing systems ranging from combustion products, to π-conjugated polymers with aromatic moieties, and graphene molecules in Materials Science. For the latter compounds Raman spectroscopy is the main vibrational spectroscopy technique usually considered, and it is an excellent tool for the characterization of graphene [2]. However, based on these findings, one can foresee that IR spectroscopy may add valuable information on the molecular structure of edges in condensed aromatic systems, to which Raman spectroscopy is less sensitive (see Fig. 2).

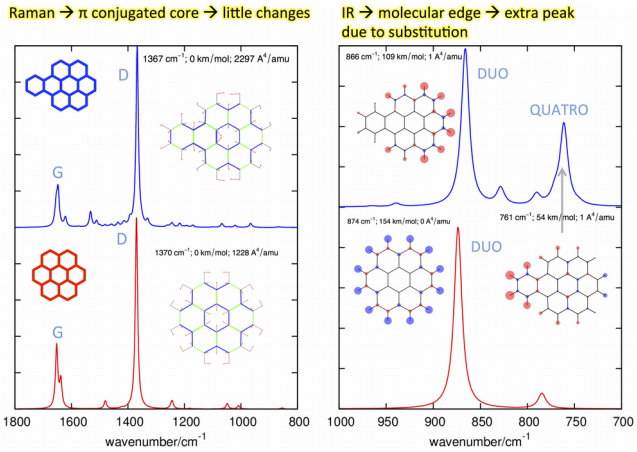


Fig.2 Slight PAH structure change mostly affects IR.

**References**

[1] M. Tommasini, A. Lucotti, M. Alfè, A. Ciajolo, G. Zerbi, Spectrochimica Acta A, 152 (2016) 134–148; https://doi.org/10.1016/j.saa.2015.07.070

[2] A.C. Ferrari, D. Basko, Nat. Nano. 8 (2013), 235; https://doi.org/10.1038/nnano.2013.46