

## From quantum topology and bond alternation to topological insulators

Julia Contreras-García<sup>a</sup>, Ángel Martín Pendás<sup>b</sup>, Francisco Muñoz<sup>c</sup>

<sup>a</sup> *CNRS-Sorbonne Universités, Laboratoire de Chimie Théorique, Paris, France*

<sup>b</sup> *Departamento de Química Física y Analítica, Universidad de Oviedo, Oviedo, Spain*

<sup>c</sup> *Departamento de Física, Facultad de Ciencias, Universidad de Chile, Santiago, Chile*

While the prediction and experimental realization of topological insulators constituted a revolution in material science, the language gap between physicists and chemists has precluded the expansion of the field in the chemical literature.

However, the main concepts involving topological insulators can be understood resorting to a slight variation of the familiar Hückel formulation and quantum topology (the quantum topology of topological insulators!).

I will dwell on the electron delocalization characteristics of this model which requires bond alternation. A bond alternation that is very problematic for DFT! So I will also show some preliminary results highlighting DFT failures in this direction.