

## SEMINAIRE EXCEPTIONNEL (CEA - SPCSI / SPEC)

**Mardi 02 Octobre 14h00**

Orme des Merisiers Salle Itzykson, Bat.774

### **Reconstruction on the Al<sub>2</sub>Cu (001) surface led by covalent bonding**

**Laura N. Serkovic Loli**

*CSIC - Universidad del Pais Vasco, San Sebastian, Spain*

*and*

*Institut Jean Lamour (UMR7198 CNRS), Nancy, France*

Surface reconstructions are generally observed on covalently bonded materials, and they are not frequent on metal surfaces. Recently, quantum calculations on the Al<sub>2</sub>Cu metallic alloy identified *covalent-like* Al-Al bonds [1]. In this study, we show that these covalent bondings are at the origin of a surface reconstruction for Al<sub>2</sub>Cu(001) [2]. The bulk structure of the Al<sub>2</sub>Cu intermetallic compound is described by graphite-like Al 6<sup>3</sup> nets [3]. The combination of both experimental methods (STM, STS, LEED, UPS, XPS) and *ab-initio* computational methods (atomic relaxations, STM simulations, electronic structure calculations) gives many arguments to match the surface plane with a bulk truncated surface model terminated by incomplete Al planes. The covalent-like interaction is highlighted by *ab-initio* calculations: the energetic cost associated with the removal of pairs of Al atoms is the lowest for the two nearest surface Al atoms.

[1] Yu. Grin et al., J. Sol. St. Chem. 179 (2006) 1707.

[2] L.N. Serkovic Loli et al., Phys. Rev. Lett. 108 (2012) 146101.

[3] H. Nowotny and K. Shubert, Z. Metallkd. 37 (1946) 17.