Contribution ID: **25** Type: **Poster**

Ab initio vibrational properties of the MXene materials functionalized by fluorine, oxygen and hydroxyl group

Monday, 14 September 2015 19:00 (2 hours)

A new family of 2D-like nano-sized binary and ternary transition metal carbides (known also as MXenes) has received significant scientific interest due to their intriguing functionalities and technological applications. Physical and chemical properties of these material can be triggered by terminating their surfaces by various adatoms or molecules. This contribution presents first-principle studies of the influence of fluorine and oxygen adatoms as well as the surface terminating OH group on the lattice dynamics of pristine Ti2C monolayers.

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Session Classification: Poster session w/ wine/beer

Track Classification: DyProSo2015 Main track