



ID de Contribution: 37

Type: **Non spécifié**

Structural and electronic properties of III-Nitrides, MoS₂ and MoSe₂: From bulk polytypes to 2D structures

lundi 12 septembre 2022 11:50 (20 minutes)

While it is well known that the III-Nitrides are the materials for the highly efficient light-emitting diodes, among other optoelectronic devices, the transition metal dichalcogenides (TMDC) also offer a great potential use in the field of 2D materials with interesting electronic and optoelectronic properties. In the case of III-Nitrides, the interest on these materials was renewed, now as a 2D material, when Tsipas and collaborators [1] found that it is possible to grow hexagonal AlN nanolayers on surfaces of Ag (111) and Al Balushi and colleagues found that hexagonal GaN can be obtained via encapsulation of graphene [2]. Moreover, in the case of TMDC, their bulk counterparts were less studied than the 2D ones, and the knowledge of their structural and vibrational properties could help to obtain better 2D samples. It is well known that the bulk structure of these materials presents polytypism, which is not yet well understood by the scientific community. The same holds in the case of III-Nitrides, which the zinblende, wurtzite and the rocksalt forms were extensively studied, and not their hexagonal closed-packed (hcp) structure. So, in this work, we report our theoretical results (with van der Waals corrections included) for the structural and vibrational properties of the bulk polytypes of MoS₂ and MoSe₂, as well as for the hcp form of III-Nitrides, extending our study to the 2D structures of these materials. For the 2H polytype of MoS₂, we have found that, the experimental measured bulk modulus is underestimated once, from our theoretical data, these measurements show a combination of hydrostatic and axial strains, which preserves the symmetry of the unit cell, due to its lubricant properties. We have also shown that, in the case of III-Nitrides, an axial strain applied to the wurtzite structure can transform it to the hexagonal closed-packed one. Going to the III-Nitrides 2D structures, we have studied the graphene-like, the square lattice and the haeckelite 8-4 ones. Our results show that the graphene-like structure is more stable one and their electronic structures show an indirect bandgap. Finally, we show our results for the structural and electronic properties of MoS₂/MoSe₂ lateral interfaces in both zig-zag and armchair configurations. Band offsets and alignment of these interfaces were also obtained. Our results have shown that the band offsets have small values, 76.0 and 23.3 meV for both zig-zag and armchair configurations, respectively. This feature favors the formation of type II superlattices and quantum wells, with good application for optoelectronic devices independent of its configuration.

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Classification de Session: Oral