UNIVERSIDADE FEDERAL DE SANTA MARIA
CENTRO DE CIÊNCIAS NATURAIS E EXATAS
PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA

Blaucius Bla

SOBRE OS BLAS DA VIDA

Santa Maria, RS
2022

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Tese apresentada ao Programa de Pós-Graduação em Física da Universidade Federal de Santa Maria (UFSM, RS), como requisito parcial para obtenção do grau de Doutor em Física.

Orientador: Profº Dr. Bleucius Ble

Santa Maria, RS
2022

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E-mail: blauciusbla@bla.com

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Aprovado em XX de Mês de XXXX:

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, Dr. (UFSM)
(Presidente/Orientador)

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, Dr. (UFSM)

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, Dr. (UFSM)

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, Dr. (EXT)

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, Dr. (EXT)

Santa Maria, RS
2022

Aos meus pais Adelar e Haidi

AGRADECIMENTOS

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Speech has allowed the communication of ideas

Enabling human beings to work together to build the impossible

Mankind's greatest achievements have come about by talking

Our greatest hopes could become reality in the future

With the technology at our disposal, the possibilities are unbounded

All we need to do is make sure we keep talking

(Talkin' Hawkin - Pink Floyd)

RESUMO

SOBRE OS BLAS DA VIDA

AUTOR: Blaucius Bla

ORIENTADOR: Profº Dr. Bleucius Ble

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Palavras-chave: bla. ble. bli. blo. blu.

ABSTRACT

ON THE BLAS OF LIFE

AUTHOR: Blaucius Bla

ADVISOR: Profº Dr. Bleucius Ble

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Keywords: bla. ble. bli. blo. blu.

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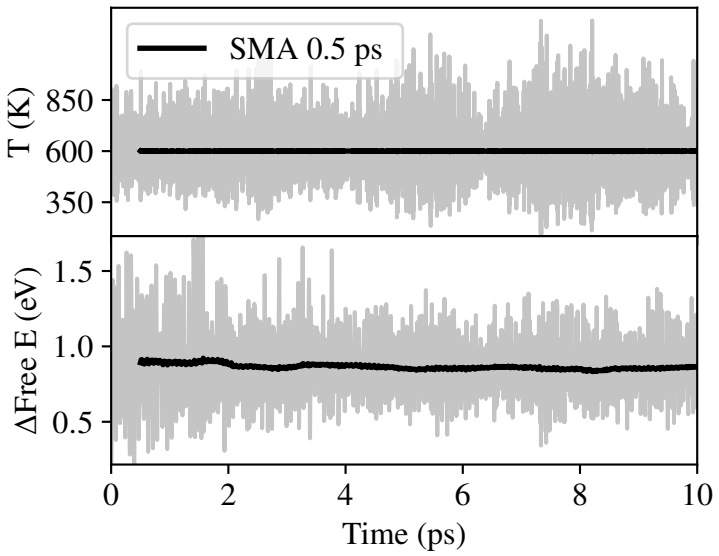
Figura 1 – legenda



Fonte: SIM FUI EU QUE FIZ

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2 GRAPHENE AND SILICENE NANODOMAINS IN A ULTRA-THIN SIC LAYER FOR WATER SPLITTING AND HYDROGEN STORAGE. A FIRST PRINCIPLE STUDY

First-principles calculations within the density functional theory (DFT) have been addressed to investigate the energetic stability, electronic and optical properties of graphene and silicene nanodomains in a SiC single layer (h-SiC). We observe that graphene domains form a planar structure and give rise to an occupied and an empty electronic levels inside the h-SiC band gap, leading the h-SiC to present a strong optical absorption peak in the visible region. On the other hand, when a silicene nanodomain is present the system is no longer planar and present a corrugated structure similar to the silicene structure. The silicene nanodomain introduce three empty electronic levels within the band gap, leading the h-SiC with optical absorption in the visible region. These results show that a graphene nanodomain in h-SiC is appropriate for optical devices, while silicene nanodomains form almost sp^3 quantum dots. This finding suggest that the graphene and silicene nanodomains in a SiC single layer increase the possibility to use h-SiC to produce new electronic and optical devices as well for energy storage by hydrogen adsorption. In fact, we study the H2 and O2 adsorption on the pristine system and on the nanodomains, we observe that the presence of the nanodomais increase the binding energies of the adsorbed molecules (KREMER; BAIERLE, 2020).

3 TWO-DIMENSIONAL NANODOMAINS AS QUANTUM DOTS MODELS IN AN ULTRA-THIN HYDROGENATED SIC LAYER

First-principles calculations within the density functional theory (DFT) are addressed to study the energetic stability and the electronic, magnetic, and optical properties of embedded nanodomains (NDs) formed by threefold coordinated Si and C atoms within a hydrogenated silicon carbide (H-SiC) monolayer. The total energy calculations show that these nanodomains have low formation energy and act as two-dimensional quantum dots (2D QDs), giving rise to localized electronic levels inside the H-SiC bandgap. The stability of the QDs is ruled by their size and shape. For NDs where the number of threefold Si and C atoms are the same, the system is a nonmagnetic semiconductor, whereas if the number of threefold coordinated Si and C atoms is different, the system is a magnetic semiconductor with a magnetic moment of 1 μ_B per unpaired (Si or C) atom present in the QDs. The calculated optical spectra show that there is a strong absorption optical in the visible region, and the position of the optical absorption peaks presents a dependence with the size and shape of the QDs. These findings are in accordance with previous works where 2D SiC QDs were investigated and the results suggest that 2D SiC QDs are potential materials for optical applications. Furthermore, our DFT results can be used to obtain 2D SiC QDs with desirable electronic, magnetic, and optical properties to be employed in nanodevices (KREMER; BAIERLE, 2021).

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KREMER, L. F.; BAIERLE, R. J. Graphene and silicene nanodomains in a ultra-thin SiC layer for water splitting and hydrogen storage. a first principle study. **International Journal of Hydrogen Energy**, Elsevier, v. 45, n. 8, p. 5155–5164, 2020.

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