

# US-Africa Initiative Workshop at APS March Meeting Sunday, March 14, 2021

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## Lecturer

Topic: Microscopic control of SiGe/high-k oxide gate stack for p-MOSFET hole qubits



## Research

My research interest involve the investigation of semiconductor materials ( e.g Full and half-Heusler alloys) properties for photovoltaic, thermoelectric and spintronic devices applications using density functional theory. Currently, I am investigating the properties of Si-SiGe-Ge alloys within the activity of the EU project iQubits "www.iqubits.eu".

## Collaboration

I have worked in collaboration as a postdoc in the group of Dr. Arrigo Calzolari at CNR-NANO, Modena.  
<http://amuse.nano.cnr.it/>

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# Microscopic control of SiGe/high-k-oxide gate stack for p-MOSFET hole qubits

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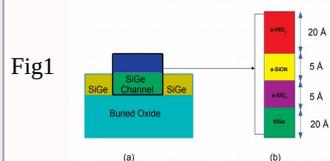
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## INTRODUCTION

The potential of silicon-based electron-spin and hole-spin coupled quantum-dot qubits as material for commercial complementary metal oxide semiconductor (CMOS) technology have generated a lot of interest due to their greater significant of record coherence times and fidelity. Despite of these characteristics, their operation has been limited to temperatures below 100 mK because of the low confinement and coupling energies. Getting qubit with higher confinement and coupling energies, with spin resonance in the upper mm-wave region will give room for higher temperature operation. Therefore, many channel materials such as Si-channel n-MOSFETs (electron-spin qubit) and SiGe-channel p-MOSFETs (hole-spin qubit) are now being investigated for the realization of quantum-dot qubits with higher temperature and fidelity for quantum computing. Thus, the control and the stability of the resulting qubits rely on the control and the stability of the underlying MOSFET device.

## METHODOLOGY



The semiconductor channel is modeled through a periodic supercell including a  $\text{Si}_{0.75}\text{Ge}_{0.25}(001)$  surface (i.e. 128 atoms) with a  $(2 \times 2)$  lateral periodicity of dimension  $(11.15 \times 11.15) \text{Å}^2$  and 11.15 Å of thickness, obtained through the geometry optimization of the  $(2 \times 2 \times 2)$  cubic supercell. A 15 Å thick layer of vacuum was added to prevent interactions between periodically repeated slab replicas. Bottom layer was passivated with Hydrogen (H).

## STRUCTURAL OPTIMIZATION

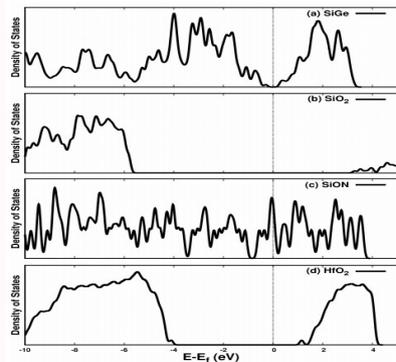
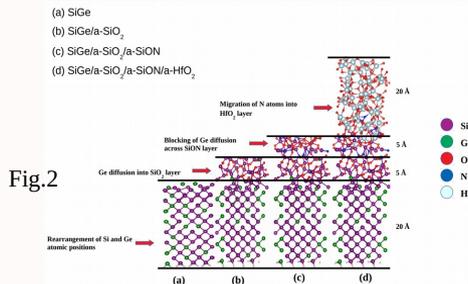


Fig.3

## RESULTS AND DISCUSSIONS

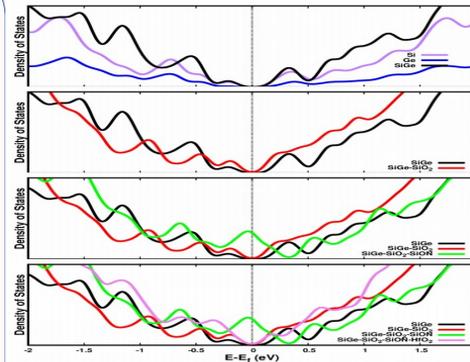


Fig.4

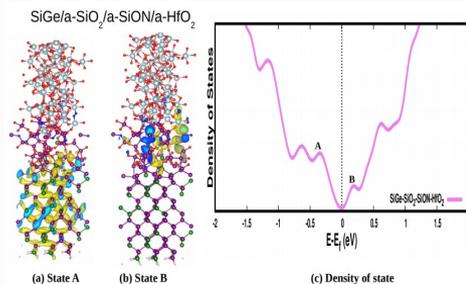


Fig.5