Unlocking the Versatile Optoelectronic Potential: Modulating Electrical properties in Silicon Clathrate films

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Abstract:

Silicon materials in their mono-, poly-, and amorphous forms have been studied in depth since they were first used in photovoltaic technologies 70 years ago. Unusual, low-density forms of silicon have recently gained attention due to attractive semiconducting and optical properties as compared to conventional silicon [1]. The type II clathrate (Na_xSi_{136}), discovered as a powder in 1965, is exciting because it is an open cage polymorph of silicon that can accommodate or release Na atoms [2]. Recently, type II clathrates in films have been explored, which is a way forward for thin film based technologies [3]. The electronic properties of these cages can be dramatically altered by adding or removing Na, which makes them useful for a variety of applications in optoelectronics and energy conversion devices. By changing the composition parameter 'x' of Na in Na_xSi_{136} films from '0' to ‘23’, the state can be changed from semiconducting to metallic. However, how exactly Na enters or exits the vacant cages of Na_xSi_{136} remains to be determined.

This research focuses on investigating the electronic properties resulting from the insertion and removal of Na atoms in Na_xSi_{136} films using Kelvin Probe-Ambient pressure photoemission spectroscopy (KP-APS) and density functional theory (DFT) calculations for the first time. Clathrate films of different thicknesses were prepared on various types of silicon wafers and pressed by press annealing to improve the overall film quality with decreasing thickness. We probed the energy levels and accurately drew the band diagram for each of the tested clathrate systems using KP-APS and optical measurements. This work highlights the great potential of processing and doping strategies for bulk clathrate films to optimize their use in photovoltaic devices with a novel heterojunction configuration, as well as their potential application in LEDs, sensors and lithium-ion batteries.

Acknowledgement

This work is financed by ANR Exosil- Exotic Silicon: silicon clathrate films (project-ANR-22-CE50-0025).

References

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