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Short communication

# Doped aluminum nanocones as an efficient electron field emitter: A first-principles investigation

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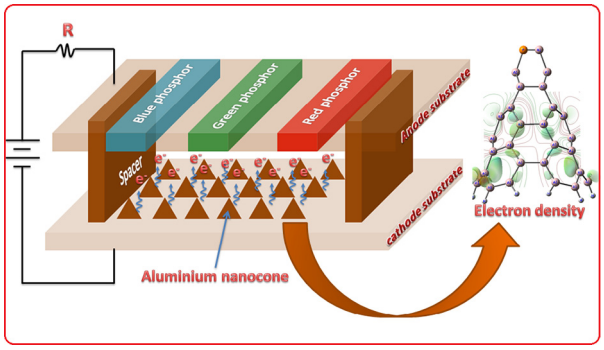
## GRAPHICAL ABSTRACT

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## ABSTRACT

We report on the basis of density functional theory, the field emission properties of pristine and doped aluminum nanocone (Al-NC). We substituted the apex of the Al-NC with group IV and group V elements, namely arsenic (As), germanium (Ge) and phosphorous (P) atoms and had carried out studies on these nanocone structures. The density of states (DOS) spectrum gives a clear perception of the charge distribution over the Al-NC surface on doping. Furthermore, the Richardson-Dushman formula has been used to correlate the work function Φ and the charge density. We have observed that doping at the apex of Al-NC leads to the variation in work function Φ. The results show that the field emission properties of Al-NC can be improved with the substitution of As, Ge, and P at the apex of the structure. Our findings suggest that doping of the Al-NC with Ge, As and P leads to the improved field emission properties, which can be used for nanoelectronics and vacuum electronics.

## 1. Introduction

The recent advancement in the micro and nanofabrication techniques are being utilized for the synthesis of one-dimensional (1D) materials such as nanorod, nanowire, nanocone that can be used for various applications such as vacuum electronics, molecular devices and optoelectronic devices [1, 2]. It is well-known that electron field emission or cold field emission is a quantum mechanical tunneling effect where the electrons across the Fermi energy level are emitted to the vacuum on applying the external electric field. Moreover, the widely accepted nanostructure for the field emission process is the 1D structure. It is known that Fowler and Nordheim formulate the accepted theory of field emission with the help of Schrödinger equation [3]. Furthermore, from the Fowler-Nordheim equation, the current density

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**Table 1**
HOMO-LUMO gap of Al-NC material with various percentages of HF exchange.

| Exchange- correlation functional | Hybrid GGA | Hybrid GGA | Hybrid GGA | Hybrid GGA | Hybrid-meta GGA |
|---|---|---|---|---|---|
| Percentage of HF exchange (X) | 20 | 21.8 | 25 | 25 | 27 |
| Nanostructure | B3LYP | X3LYP | PBE0 | B1LYP | M-06 |
| Al-NC | 0.51 | 0.56 | 0.67 | 0.68 | 0.75 |
| Al-NC-As | 0.5 | 0.54 | 0.64 | 0.66 | 0.73 |
| Al-NC-Ge | 0.63 | 0.68 | 0.7 | 0.73 | 0.79 |
| Al-NC-P | 0.5 | 0.54 | 0.63 | 0.66 | 0.71 |

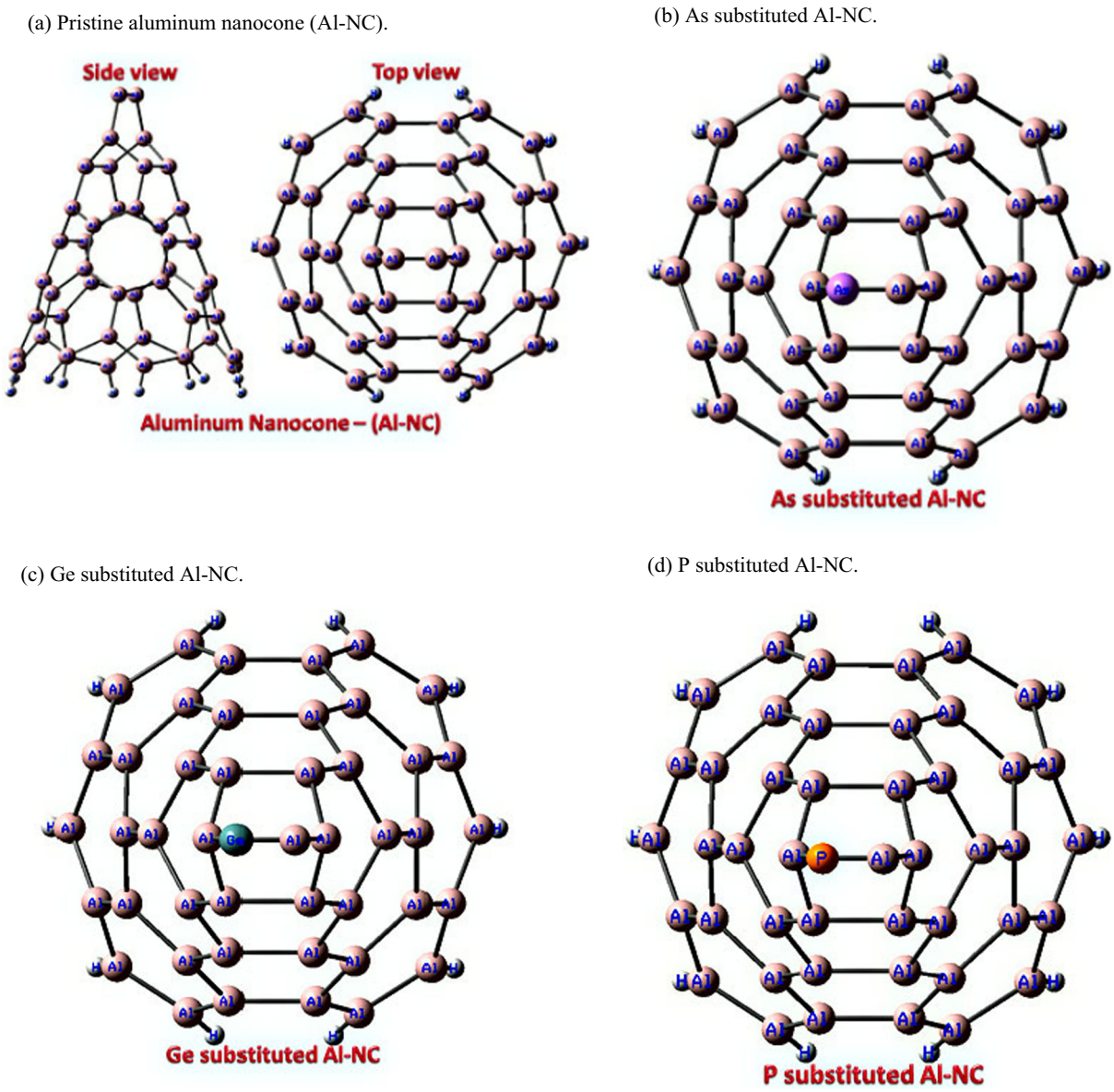


**Fig. 1.** Schematic diagram of pristine and doped aluminum nanocone.

of the field emitting source depends on the work function Φ and the field enhancement factor β [4]. Moreover, the known fact is that the excellent field emission material should have a low work function that depends upon the size and shape of the nanomaterial. Besides, the previous reports show that ZnO nanostructures, carbon-based materials such as carbon nanotubes have been utilized for field emission [5–7]. Among 1D material, CNTs are widely studied owing to their excellent thermal conductivity, high mechanical strength, and excellent electrical conductivity. Also, CNT based field emitters possess low turn on, high current density and threshold electric field [8–10]. Apart from CNT, other nanomaterials such as boron nitride and aluminum nitride are also used as robust field emitters at ambient conditions [11–14]. Peyghan group [15–18] have extensively studied the interaction behavior of various gas molecules namely $NO_2$, CO, $NH_3$, and nitrous oxide on different nanostructures of AlN such as nanocone, nanotube and nanosheet using density functional theory (DFT) method based on charge transfer.

The metallic nanocones have been synthesized by various methods, namely electron beam evaporation, thin-film metallization, UV-nanoimprint lithography, and argon ion milling [19, 20]. Moreover, if we