Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Supplementary Information - Chemical and substitutional doping, anti-site and vacancy formation in monolayer AlN and GaN

Yelda Kadioglu,[a,b] Fatih Ersan,[a,b] Deniz Kecik,[b,c] Olcay Üzengi Aktürk,[d,e] Ethem Aktürk[f,e*] and Salim Ciraci [b‡]

Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

We present some extra datas related with the results in the main text as below.

1. Energy bands of patterned structures consisting of single adatom adsorbed to each periodically repeating (2×2) supercells of h-AlN and h-GaN. These patterned structures can attain either half-metallic bands as shown in Fig. 5 in the main text, or magnetic metals or magnetic semiconductors with different band gaps for different spin-directions as in this supplementary material (Fig.S1).
2. Stable hydrogenation geometries of h-AlN and h-GaN were described in Fig.9 in the main text. In this supplementary materials (Fig.S2) we present details about the specific hydrogenation geometries, which lead to dynamical instabilities.
3. The prime configurations of H_2 and O_2 dissociating at the cation vacancy site were presented in Fig. 11 in the main text. In this supplementary material (Fig.S3-S6) we present other configurations of approach of H_2 and O_2 molecules, which lead to dissociation and physisorption.

[a] Department of Physics, Adnan Menderes University, Aydın 09010, Turkey.
[b] Department of Physics, Bilkent University, Ankara 06800, Turkey.
[c] UNAM-Institute of Materials Science and Nanotechnology, University, Ankara 06800, Turkey
[d] Department of Electrical and Electronic Engineering, Adnan Menderes University, 09100 Aydın, Turkey
[e] Nanotechnology Application and Research Center, Adnan Menderes University, Aydın 09010, Turkey
* Fax: +902562135379; Tel: +902562130835; E-mail: ethem.akturk@adu.edu.tr
‡ E-mail: ciraci@fen.bilkent.edu.tr

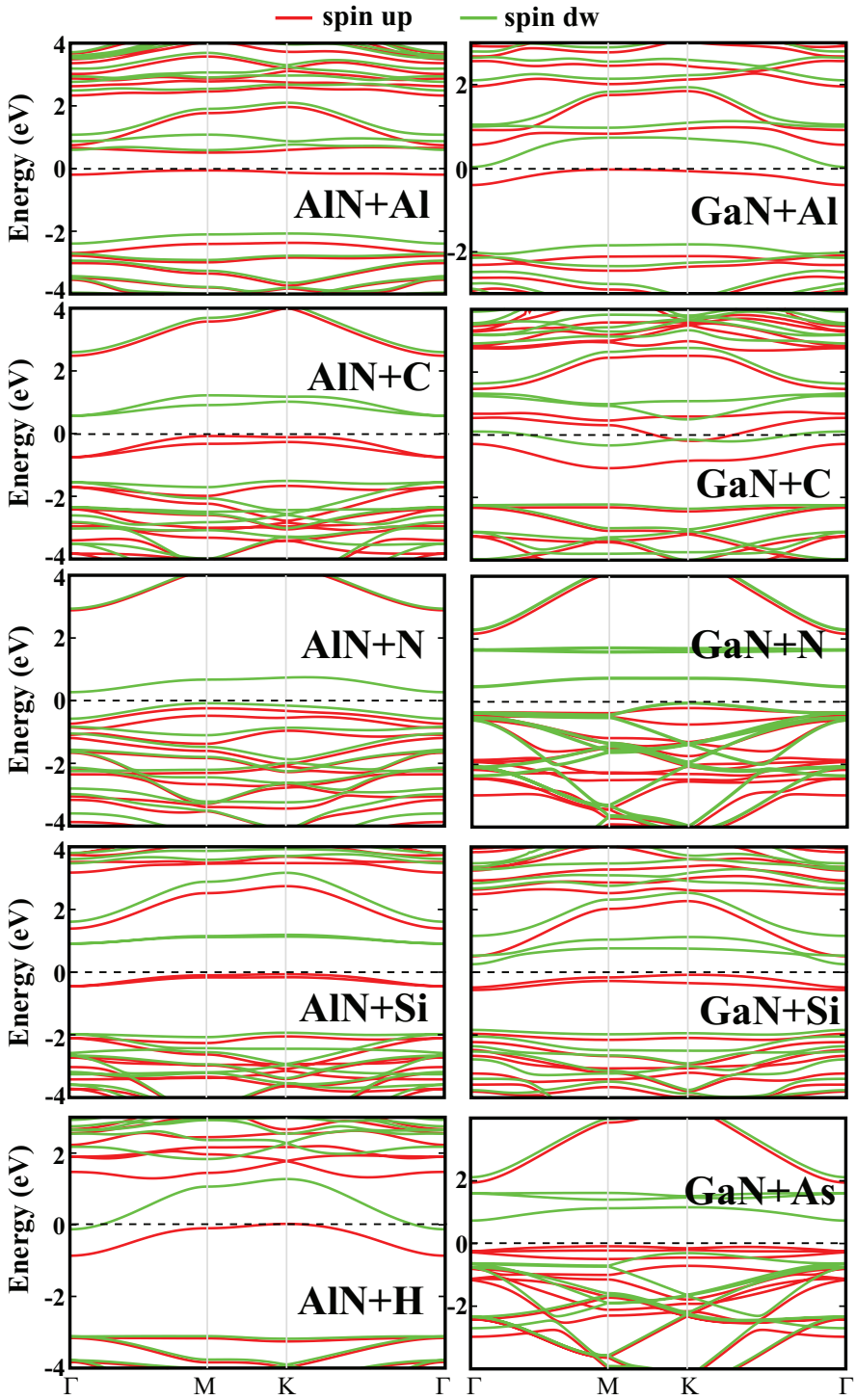

Fig. 1 Left panels: Energy bands of patterned structures of a single adatom (Al, C, N, Si, H) adsorbed to each periodically repeating (2×2) supercell of h-AlN monolayer. Zero of energy is set at the Fermi level. C, N and Si adatoms give rise to magnetic semiconductors, which have different band gaps for different spin-direction. Right panels: Same for h-GaN with adatoms Al/Ga, C, N, Si and As, each forming a patterned (2×2) structure.

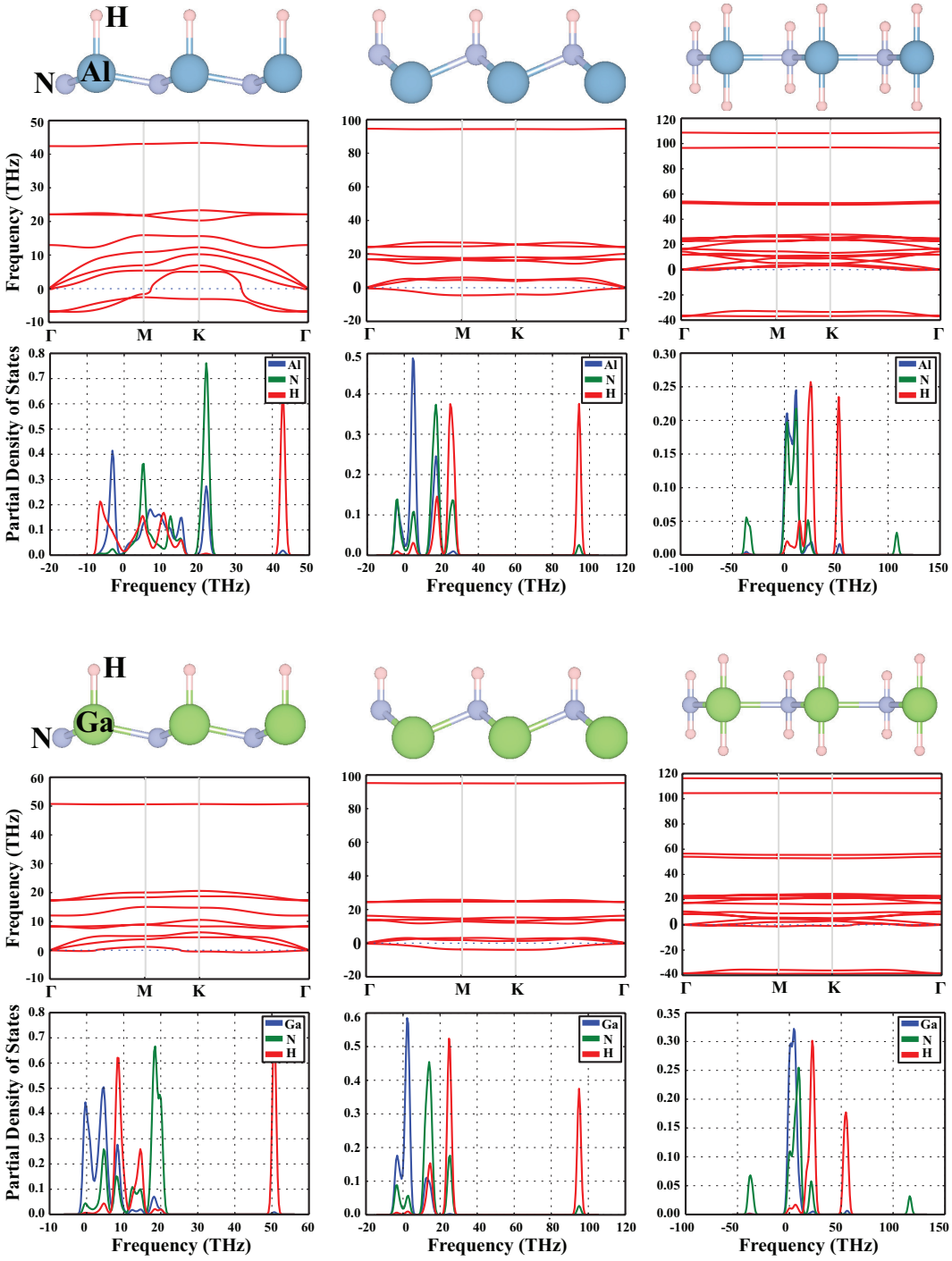

Fig. 2 Various hydrogenation configurations of h-AlN and h-GaN which leads to dynamical unstabilities. Top panels: Hydrogenation geometry of h-AlN, phonon dispersion curves with imaginary frequencies, atom projected densities of states. Bottom panels: Same for h-GaN.

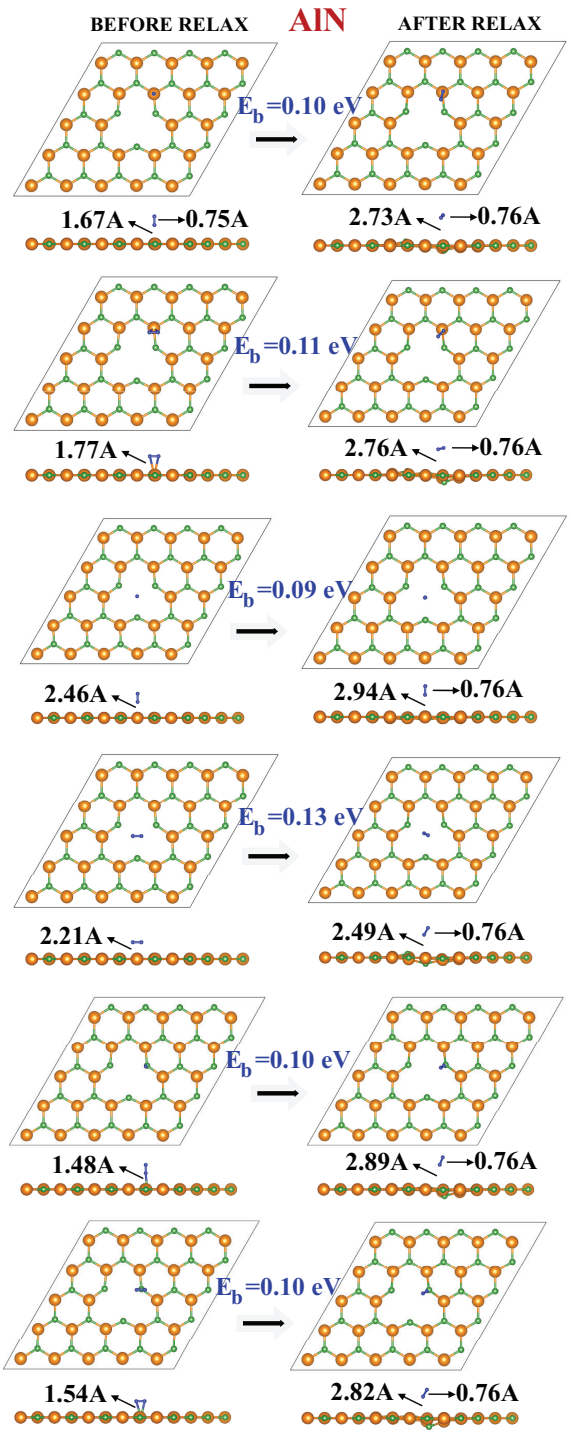

Fig. 3 Left: Top and side views of various configurations of H_2 approaching the cation vacancy site of h-AlN. Right: Optimized configurations with relevant structural parameters and energetics for physisorption or dissociation energies.

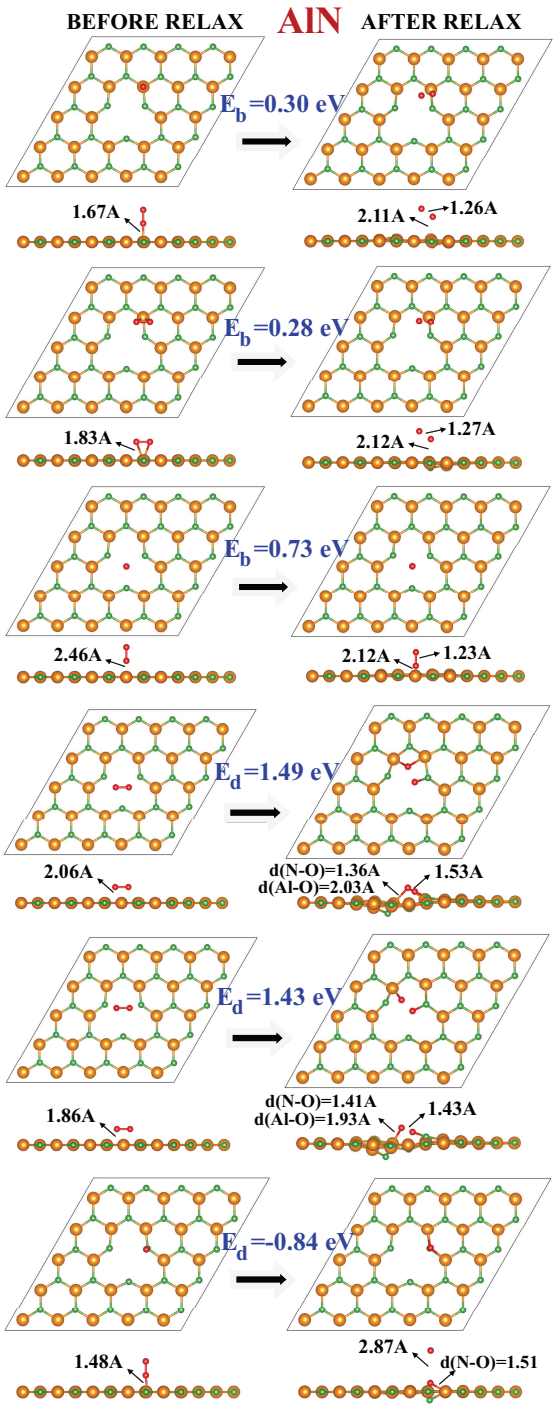

Fig. 4 Left: Top and side views of various configurations of O_2 approaching the cation vacancy site of h-AlN. Right: Optimized configurations with relevant structural parameters and energetics for physisorption or dissociation energies.

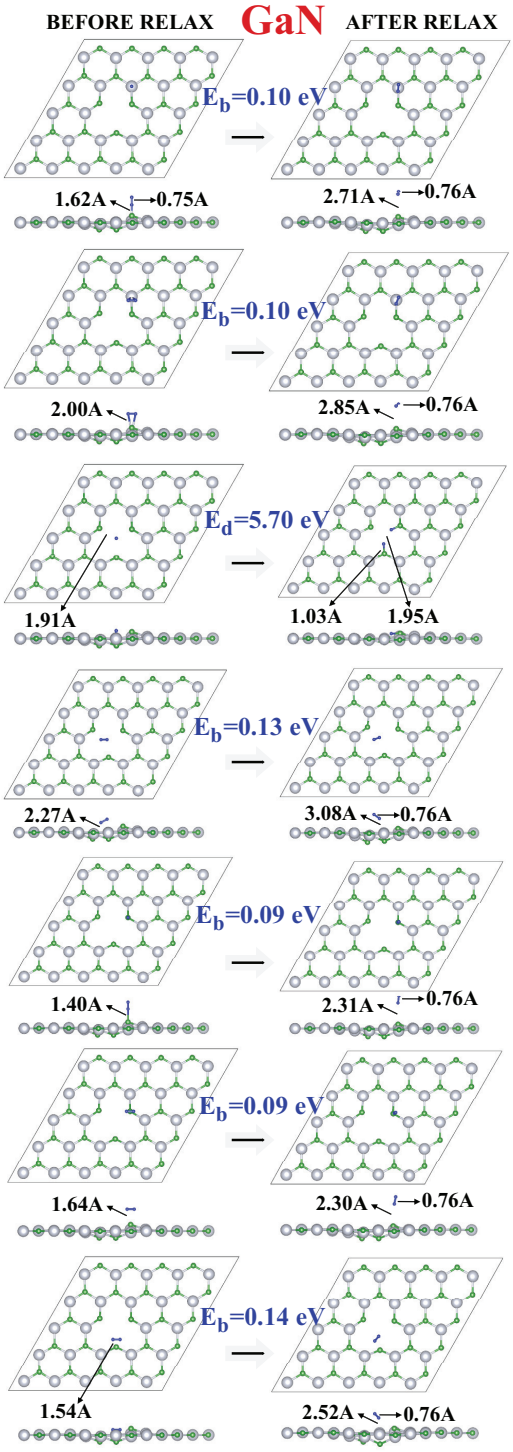

Fig. 5 Left: Top and side views of various configurations of H_2 approaching the cation vacancy site of h-GaN. Right: Optimized configurations with relevant structural parameters and energetics for physisorption or dissociation energies.

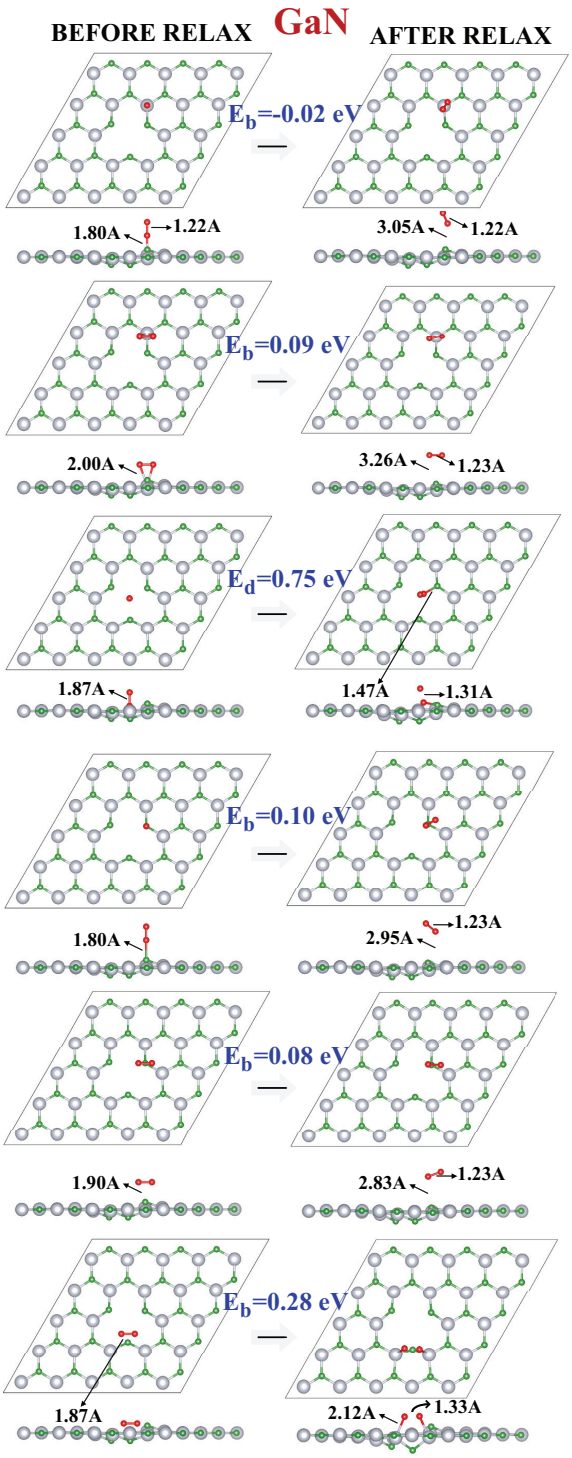

Fig. 6 Left: Top and side views of various configurations of O_2 approaching the cation vacancy site of h-GaN. Right: Optimized configurations with relevant structural parameters and energetics for physisorption or dissociation energies.