Low-density nanoporous phases of group-III nitrides built from sodalite cage clusters

Zhifeng Liu\textsuperscript{a}, Xinqiang Wang\textsuperscript{a}, Gaobin Liu\textsuperscript{a}, Ping Zhou\textsuperscript{a,b}, Jian Sui\textsuperscript{a}, Xuefang Wang\textsuperscript{a}, Hengjiang Zhu\textsuperscript{c} and Zhilin Hou\textsuperscript{d}

\textsuperscript{a} College of Physics, Chongqing University, Chongqing, P.R. China.

\textsuperscript{b} School of Science, Chongqing Jiaotong University, Chongqing, P.R. China.

\textsuperscript{c} College of Physics and Electronic Engineering, Xinjiang Normal University, Urumchi, P.R. China.

\textsuperscript{d} Southwest China Institute of Electronic Technology, Chengdu, P.R. China.

*Corresponding Author: Fax: +86-023-65678365; Tel: +86-023-65678365; E-mail: xqwang@cqu.edu.cn

S1. Natural tilings of the new nanoporous phases of MN

\textbf{SOD-MN} \hspace{1cm} Pm\textsuperscript{3}n

\textbf{Face symbol:} \hspace{1cm} [4\textsuperscript{6}, 6\textsuperscript{8}]

\textbf{V, E, F:} \hspace{1cm} (24, 36, 14)

\textbf{Symmetry:} \hspace{1cm} m\textsuperscript{3}
LTA-MN  \( Fm\bar{3}c \)

Face symbol: \([4^6]\) \([4^6.6^8]\) \([4^{12}.6^8.8^6]\)

V, E, F: (8, 12, 6) \( (24, 36, 14) \) \( (48, 72, 26) \)
Symmetry: \( \overline{4}3m \) \( m\bar{3} \) \( 432 \)

FAU-MN  \( Fd\bar{3} \)

Face symbol: \([4^6.6^2]\) \([4^6.6^8]\) \([4^{18}.6^4.12^4]\)

V, E, F: (12, 18, 8) \( (24, 36, 14) \) \( (48, 72, 26) \)
Symmetry: \( \overline{3}m \) \( m\bar{3} \) \( 23 \)

EMT-MN  \( P\bar{3}1c \)

Face symbol: \([4^6.6^2]\) \([4^6.6^8]\) \([4^{15}.6^2.12^3]\) \([4^{21}.6^6.12^5]\)

V, E, F: (12, 18, 8) \( (24, 36, 14) \) \( (36, 54, 20) \) \( (60, 90, 32) \)
Symmetry: \( \overline{3}m \) \( m\bar{3} \) \( 32 \)

Tri-MN  \( R\bar{3} \)

Face symbol: \([4^6.6^2]\) \([4^6.6^8]\)

V, E, F: (12, 18, 8) \( (24, 36, 14) \)
Symmetry: \( \overline{3}m \) \( m\bar{3} \)
S2. Estimations of pore volume and specific surface area for the new nanoporous phases

From the natural tilings, one can find that the structure type is “Cage” for all of the eight new nanoporous phases. We believe, therefore, that the volume of a sphere may effectively describe the hollow space of the cage. To choose a rational radius for the sphere of the cage, we use Helium molecules Heₙ (2-10) to fill the hollow space of Mₑ₂N₁₂. After full optimization without any symmetry constraint, we find that the sodalite cage can be well retained when n≤8 and n≤6 for Ga₁₂N₁₂ Al₁₂N₁₂, respectively. Based on these calculations, the effective radius (R) of the sphere can
be defined (approximately) as: $R = R_{\text{max}} - D_m$ [see Fig. S2(a)]. In Fig. S2(b), we demonstrate how to measure the $R_{\text{max}}$ for the different cages.

Consequently, pore volume ($V_p$) and specific surface area ($S_a$) can be estimated by following equations:

$$V_p = \frac{4}{3} \pi \sum_{i} \alpha_i R_i^3$$

$$S_a = \frac{4\pi \sum_{j} \beta_j R_j^2}{m'}$$

It is important to note that our calculated results are just based on the crystal structure rather than adsorption isotherms which should consider the pressure and temperature. However, it does reflect the porosity of the new nanoporous phases to a certain extent.