Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Prediction of C_7N_6 and C_9N_4: Stable and strong porous carbon-nitride nanosheets with attractive electronic and optical properties

Bohayra Mortazavi[*a], Masoud Shahrokhi[b], Alexander V Shapeev[c], Timon Rabczuk[d] and Xiaoying Zhuang[a]

[a]*Institute of Continuum Mechanics, Leibniz Universität Hannover, Appelstraße 11, 30157 Hannover, Germany.*

[b]*Department of Physics, Faculty of Science, Razi University, Kermanshah, Iran.*

[c]*Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Nobel St. 3, Moscow 143026, Russia.*

[d]*College of Civil Engineering, Department of Geotechnical Engineering, Tongji University, Shanghai, China.*

*E-mail: bohayra.mortazavi@gmail.com

1. Atomic structures of constructed monolayers unit-cells in VASP POSCAR.

2- AIMD results for the thermal stability.

3- Failure mechanism upon the uniaxial loading.

4- HSE06 results for the total electronic density of states.

1. Atomic structures of constructed monolayers unit-cells in VASP POSCAR.

1.1-C7N6

```
  1.00000000000000
    6.7943948564804693    0.0000000000000000    0.0000000000000000
    3.3971974282402351    5.8841185491832784    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0000000000000000
  C    N
    7    6
Direct
  0.9998100576047193  0.0002509396813224  0.5000000000000000
  0.9331640163519950  0.7159702217766863  0.5000000000000000
  0.9331204068991781  0.3511955830278453  0.5000000000000000
  0.7155979589857679  0.9335029314294445  0.5000000000000000
  0.7155586812735208  0.3512017827147176  0.5000000000000000
  0.3507638336030467  0.9335002995972488  0.5000000000000000
  0.3507380370779813  0.7159747027046279  0.5000000000000000
  0.1110737155275103  0.1115015469972604  0.5000000000000000
  0.1110716970172021  0.7777302000807538  0.5000000000000000
  0.9928516147958462  0.5037223459642206  0.5000000000000000
  0.7772919263856721  0.1115054214509428  0.5000000000000000
  0.5034145543584359  0.9930456207717029  0.5000000000000000
  0.5032887640754495  0.5037339139401453  0.5000000000000000
```

1.2-C9N4

```
  1.00000000000000
    6.8747763944394347    0.0000000000000000    0.0000000000000000
    3.4373881972197169    5.9537310029223516    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0000000000000000
  C    N
    9    4
Direct
  0.9393400458179499  0.7131257480603921  0.5000000000000000
  0.9393001191584816  0.3477474643952050  0.5000000000000000
  0.7127859420819433  0.9397274414772028  0.5000000000000000
  0.7128273967788488  0.3477398726273222  0.5000000000000000
  0.3473822033077525  0.9397377476090796  0.5000000000000000
  0.3474029143193675  0.7131344478612078  0.5000000000000000
  0.1122806251630522  0.1126744582075219  0.5000000000000000
  0.1122974051619892  0.7752802886217438  0.5000000000000000
  0.7749246449094613  0.1126685991057670  0.5000000000000000
  0.9959374896874280  0.5021250988652426  0.5000000000000000
  0.5017923976542491  0.9963276492876858  0.5000000000000000
  0.5018066045797767  0.5021285977240453  0.5000000000000000
  0.9998464096288657  0.0001947787100747  0.5000000000000000
```

1.3-C10N3
1.00000000000000
6.9479592820170710 0.0000000000000000 0.0000000000000000
3.4739796410085360 6.0171092426870594 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
C N
10 3
Direct
0.9998618242113650 0.0001915034646203 0.5000000000000000
0.9421341773494589 0.7110490657941355 0.5000000000000000
0.9421032766220279 0.3470382183706917 0.5000000000000000
0.7107023464341822 0.9425717864329997 0.5000000000000000
0.7107678193893250 0.3469847987877088 0.5000000000000000
0.3466836888252871 0.9425567476066306 0.5000000000000000
0.3467199055403896 0.7109873132782667 0.5000000000000000
0.1136681523335525 0.1141695712157755 0.5000000000000000
0.1136820138782042 0.7724426820622625 0.5000000000000000
0.7719589577274917 0.1141792480925332 0.5000000000000000
0.9832906640111574 0.5084824128072398 0.5000000000000000
0.5080726875267416 0.9837057033943637 0.5000000000000000
0.5080998301508259 0.5084764676927023 0.5000000000000000

2- AIMD results for the thermal stability.

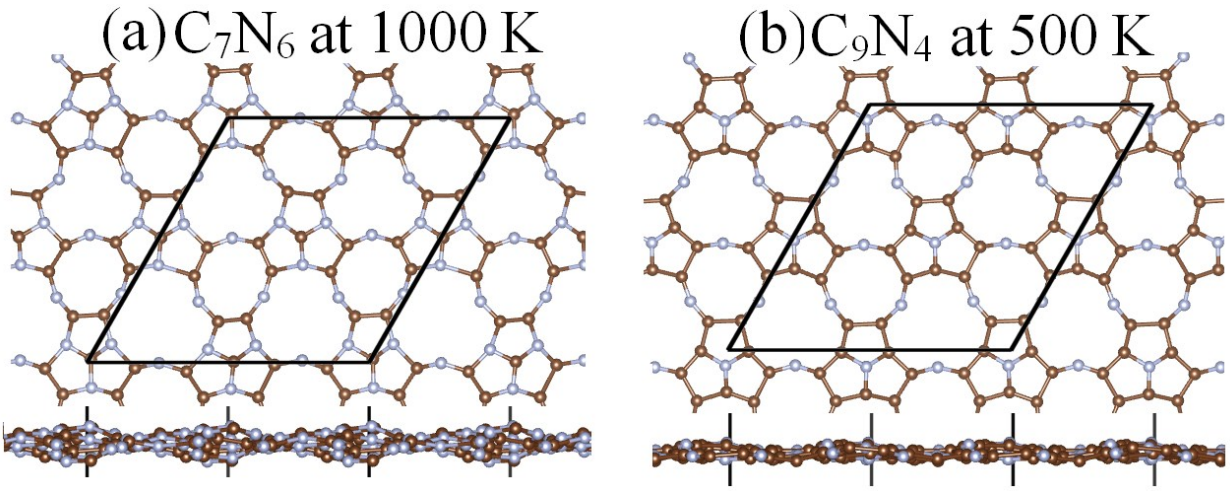

Fig. S1, Top and side views of C_7N_6 and C_9N_4 monolayers after the AIMD simulations for 20 ps.

3- Failure mechanism upon the uniaxial loading.

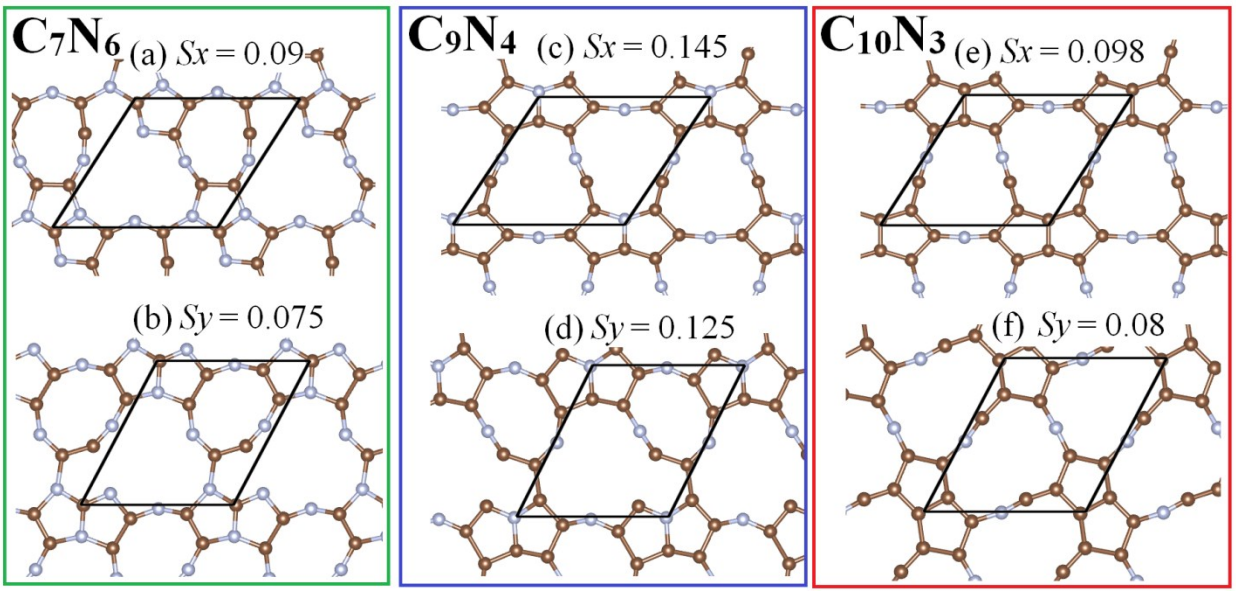

Fig. S2, Top views of the single-layer C_7N_6, C_9N_4 and $C_{10}N_3$ at strain levels shortly after the ultimate tensile strength point. S_x and S_y depict the strain levels for the uniaxial loading along the x than y directions, respectively

4- HSE06 results for the total electronic density of states.

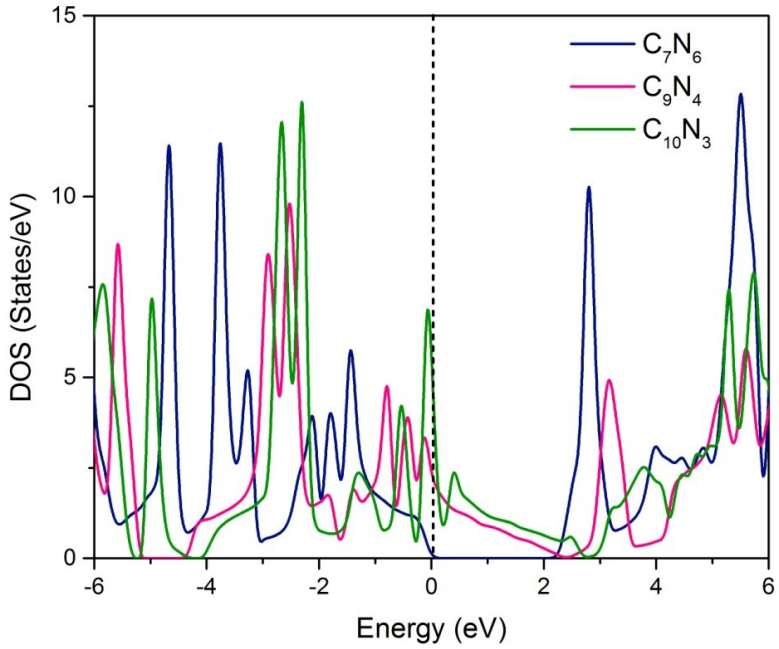

Fig. S3, Total electronic density of states predicted by the HSE06 functional. The Fermi energy is aligned to zero.