Supporting Information

Prediction of a Novel 2D Porous Boron Nitride Material with Excellent Electronic, Optical and Catalytic Properties

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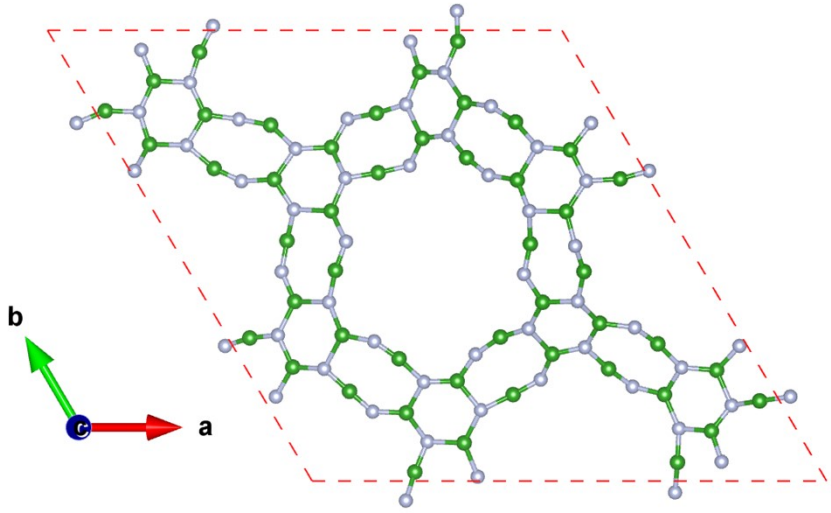

Fig. S1 Molecular dynamics snapshot of the monolayer BN-HGY after keeping the structure in a canonical ensemble for 5 ps time duration at 1000 K.

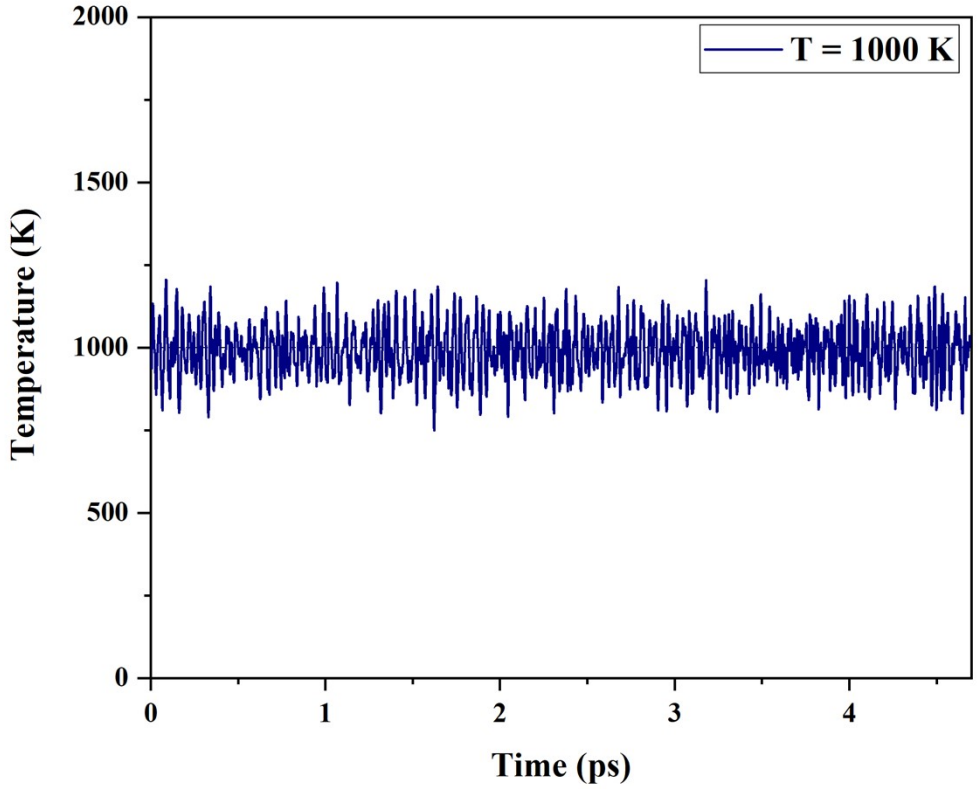

Fig. S2 Temperature fluctuations in the monolayer BN-HGY after keeping the structure in a canonical ensemble for 5 ps time duration at 1000 K.

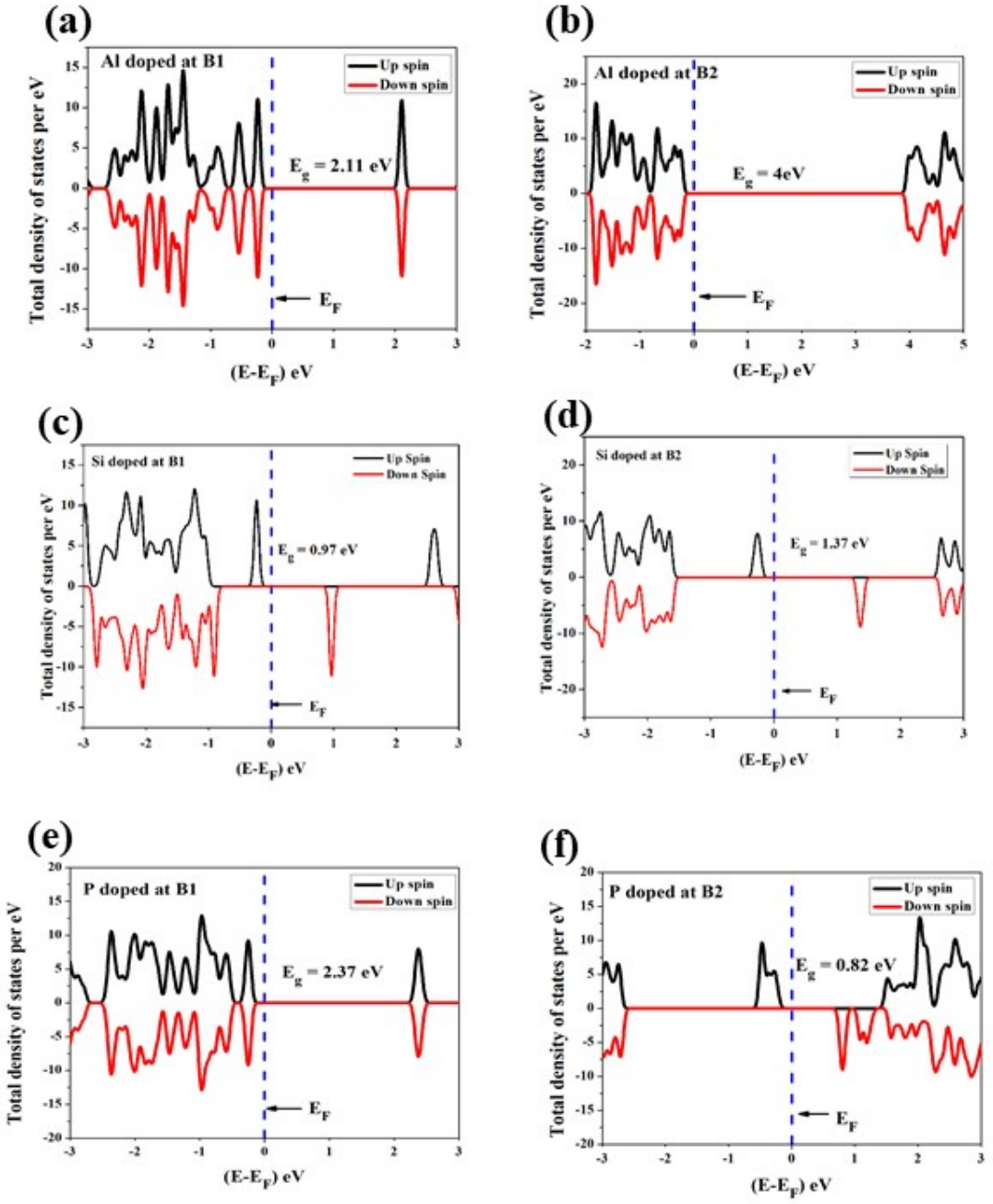

Fig. S3 Total density of states of BN-HGY with (a) Single aluminum atom doped at sp-hybridized boron atom (b) Single aluminum atom doped at sp^2-hybridized boron atom (c) Single silicon atom doped at sp-hybridized boron atom (d) Single silicon atom doped at sp^2-hybridized boron atom (e) Single phosphorus atom doped at sp-hybridized boron atom (f) Single phosphorus atom doped at sp^2-hybridized boron atom. E_F represents the Fermi level.

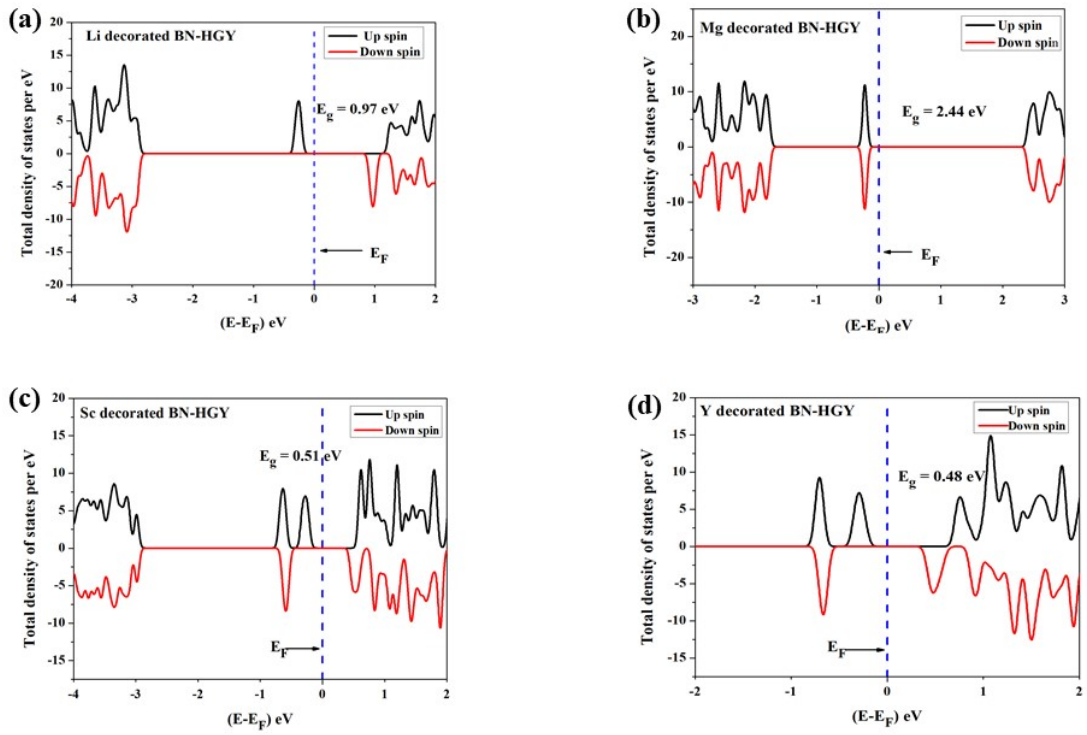

Fig. S4 Total density of states of (a) Li decorated BN-HGY (b) Mg-decorated BN-HGY (c) Sc-decorated BN-HGY (d) Y-decorated BN-HGY. E_F denotes Fermi energy.

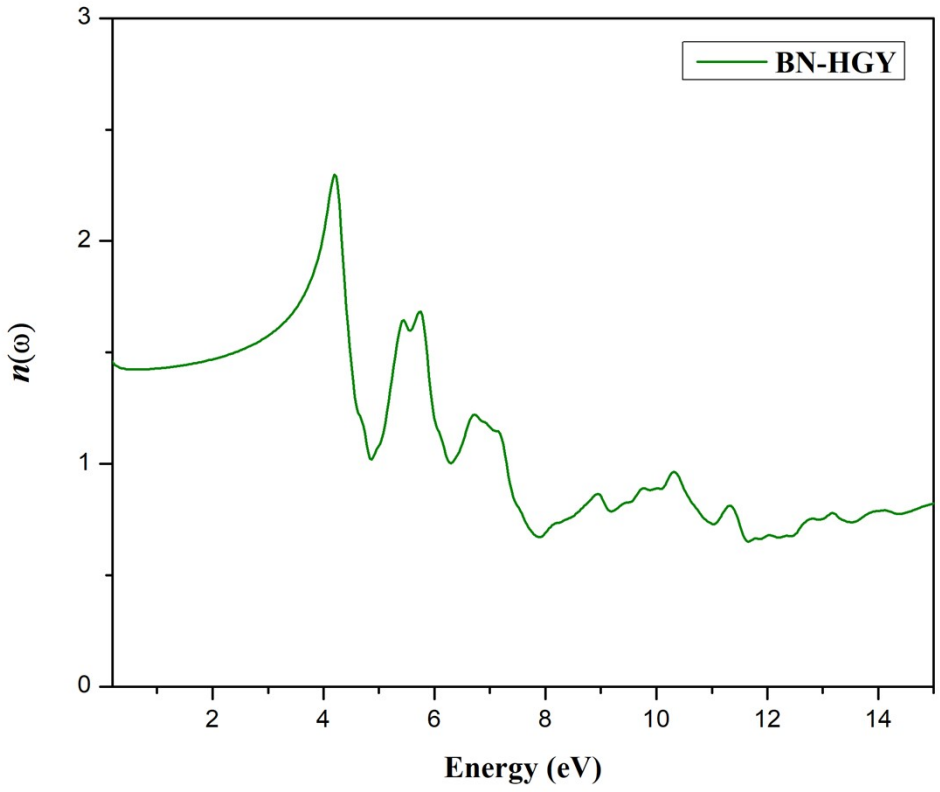

Fig. S5 The refractive index plot of the BN-HGY structure with respect to the energy of incident photon.

Structural files:

1. **Position of atoms in BN-HGY unit cell**

BN-HGY

1.00000000000000

10.9187088012999993 0.0000000000000000 0.0000000000000000

-5.4644601315000001 9.4615217934999993 0.0000000000000000

1.3044178647000000 0.7099982333000000 7.5775218135999998

B N

12 12

Direct

0.0566971741682597 0.6389019931994668 0.5018388516514525

0.1926874521823643 0.5241284730690586 0.5012197681296378

0.3218171424157124 0.7982716503003187 0.5016855801975619

0.4669220795893775 0.6691744218433832 0.5018387624006801

0.5725211902550887 0.9341637378051905 0.5019189730254173

0.3519706552889871 0.4184862157155985 0.5012359759626668

0.6353967778918047 0.5757821353811766 0.5022334759707305

0.5204436674834406 0.3250939335024693 0.5015809636535463

0.7947645531143873 0.4701586566270122 0.5016157812398711

0.6655779729666641 0.1960166681748829 0.5016103778809397

0.4147832580016411 0.0600643152078548 0.5018746838700133

0.9307550666637444 0.3553966042863624 0.5010272359740948

0.3226075156284158 0.9275871673930171 0.5018549750617227

0.1939316097735876 0.6610441430644834 0.5014884701381875

0.0632850876362697 0.3956218344595660 0.5009678428583562

0.4575531243243695 0.7970143007302519 0.5017688523523787

0.3300044546311929 0.5335609467509147 0.5011614047239463

0.3919623584420341 0.3260800870234892 0.5013022215545587

0.5953149394131602 0.6681437310394783 0.5027267575151194

0.6574528424741708 0.4607432088436683 0.5017602759131905

0.5297974545867215 0.1972455870458008 0.5016512609867482

0.7935621599514922 0.3332835057476856 0.5011492330039808

0.6646755723940350 0.0666394356041891 0.5020633883436865

0.9241158907230623 0.5986472471846720 0.5021248875915024

2. BN-HGY (2*2 supercell) coordinates after keeping the system in canonical ensemble for 5 ps at 1000 K

BN-HGY

1.00000000000000

21.8331655023710773 -0.0047829008094971 0.4308794721713001

-10.9265132170076207 18.9244222155918465 -0.0197986828702134

1.1546515469311316 0.6312696178755490 7.6087265711826575

B N

48 48

Direct

0.2036281492551567 0.0280764654485088 0.5710222100559605

0.2678061777307291 0.4643846405387267 0.6190915756682150

0.3050929325133986 0.2802539647389553 0.6109439486508895

0.1593161314111343 0.2034104530422128 0.6294810597982207

0.4601938521841759 0.1699757458804616 0.5871644829483099

0.0120527634950182 0.3207585580176112 0.5451805408171497

0.0779108853492657 0.2655464486561769 0.6175311741872769

0.3998220157295607 0.2337576299447987 0.6082082295976003

0.2171669001141310 0.3288617985019516 0.6211106889710546

0.2464222545365977 0.1593845209284770 0.6088194660204741

0.1439034117663819 0.3988898743237075 0.6343725685998401

0.3267680840811488 0.0899948261509044 0.5984998634633708

0.7166385103849671 0.0303083269181663 0.3885215117849110

0.7910841738411020 0.4566833139316616 0.4373179960059701

0.8105390596525683 0.2826980347021949 0.4124203619663437

0.6773419015502127 0.2076077775290202 0.4228284503828545

0.9563639452784801 0.1822345783922670 0.5333618461010741

0.5369227819712191 0.3259767688038166 0.5080955701484026

0.5935168386436719 0.2610353533244100 0.4899391430391826

0.8836183682436183 0.2324242740242426 0.5019601770464384

0.7334086942150361 0.3329624053219402 0.4163936018948027

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0.3379264833966513 0.7980946130787244 0.4718321772605788

0.1806219789210946 0.7133700955443698 0.4889208536587170

0.4678930938348433 0.6843672120911711 0.4860767644415845

0.0261931503448799 0.8196054729276446 0.5132817118855684

0.1031525182473200 0.7727910104485824 0.5238412446345054

0.4026791851676162 0.7339669915735516 0.5004788752570800

0.2425357693111955 0.8405513129005128 0.4698954114118827

0.2702225984302101 0.6668874055367587 0.5195672250911293

0.1617921287580946 0.9019915949527576 0.5223868605061228

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