# Global Optimization of Restructured Ga48N50
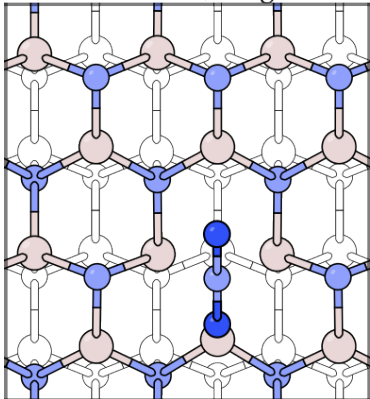
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1. From direct BLDA sampling with random rattling of 0.1 Angstrom and Hookean pre-optimization.

2. The same-element probability penalty is set to 50%, and desorbed N_2 structures are filtered out.

3. Color code: Ga - light brown; N - blue.

4. For clarity, the constrained atoms are drawn in white, and the buffer atoms are drawn in shallow color.
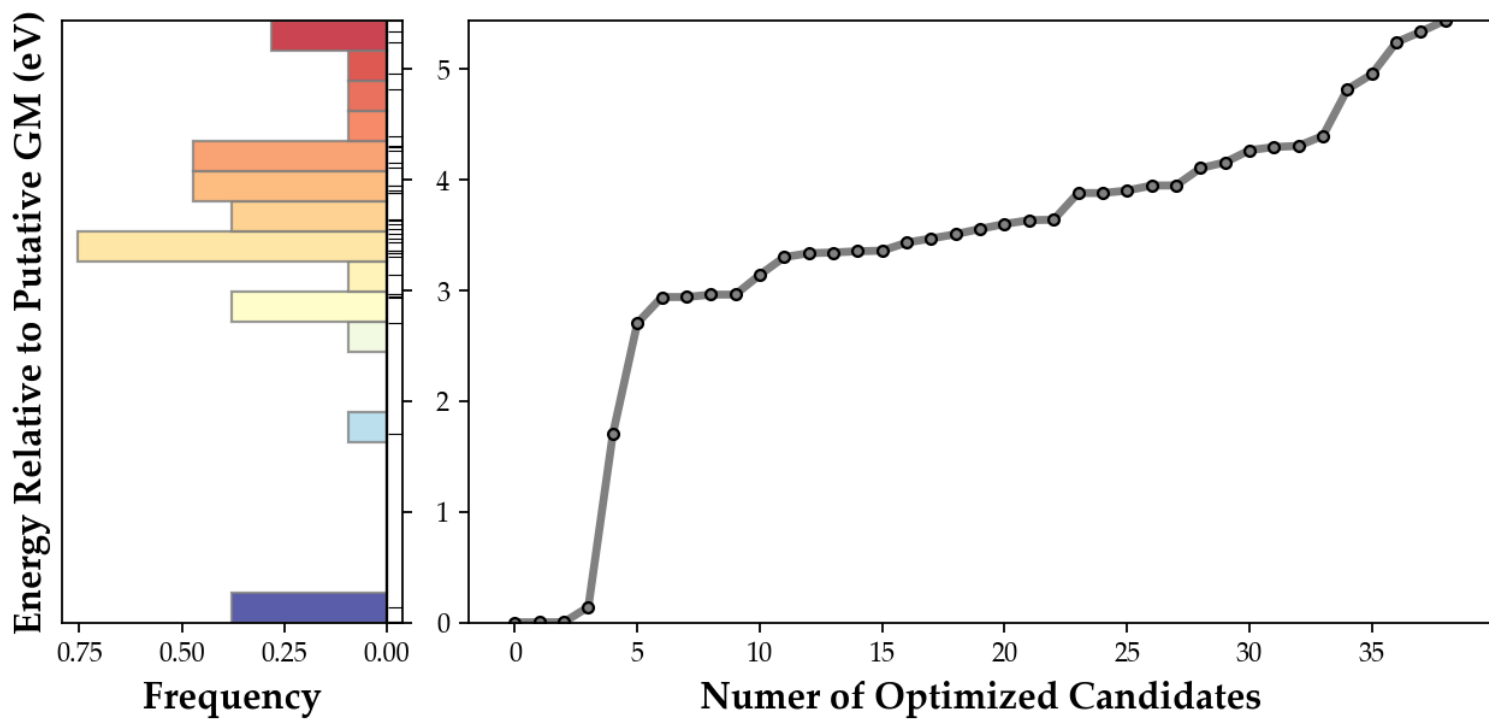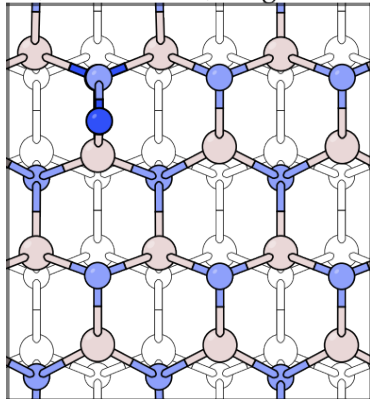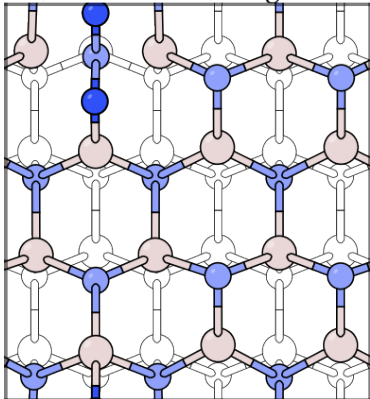
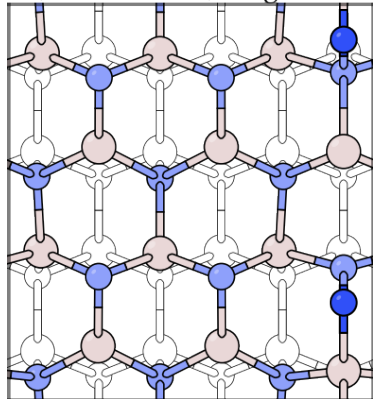#1, E = 0.000 eV, mag = -0.00　　#2, E = 0.138 eV, mag = -0.00　　#3, E = 1.700 eV, mag = 0.00　　#4, E = 2.704 eV, mag = -3.96
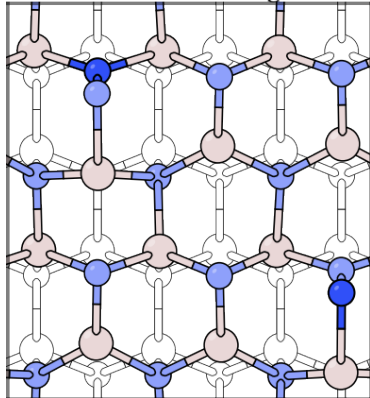
#5, E = 2.939 eV, mag = 0.00　　#6, E = 3.139 eV, mag = 0.06　　#7, E = 3.335 eV, mag = 2.57　　#8, E = 3.342 eV, mag = 2.00
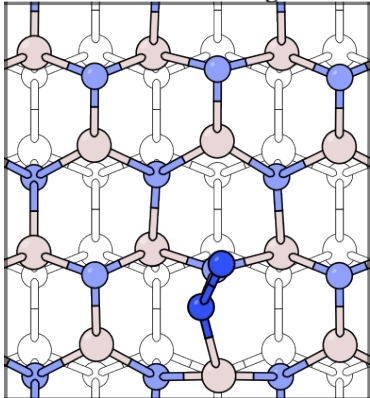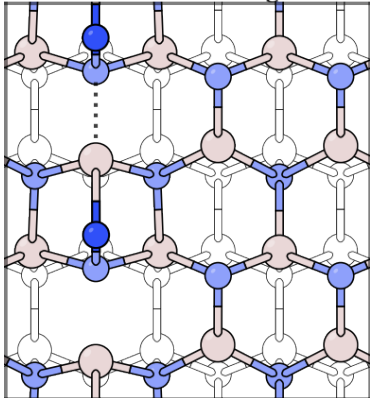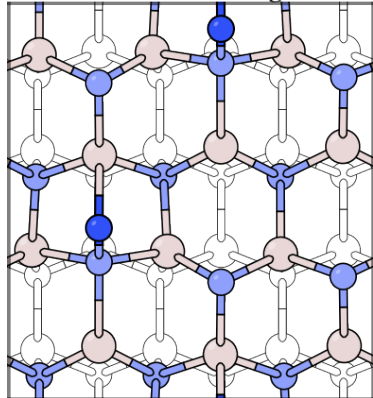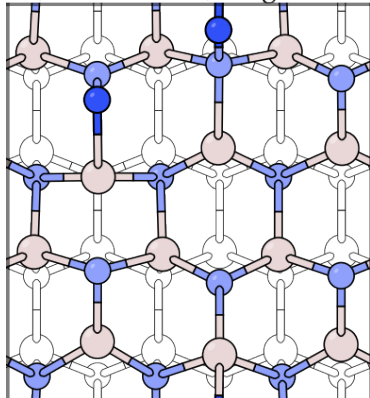
#9, E = 3.358 eV, mag = -0.00　　#10, E = 3.468 eV, mag = 2.00　　#11, E = 3.507 eV, mag = -0.00　　#12, E = 3.600 eV, mag = 1.99
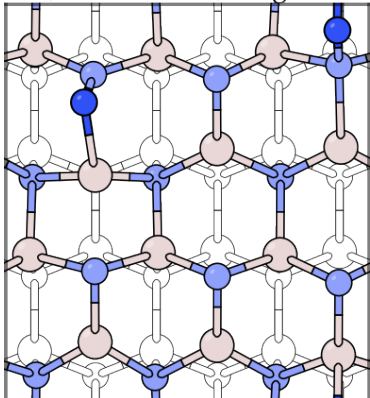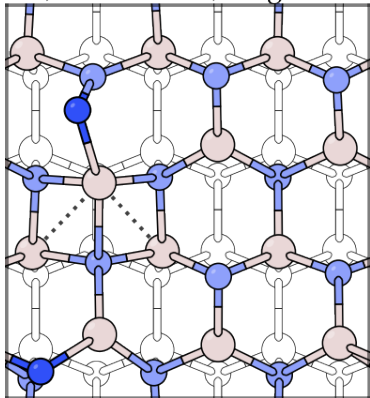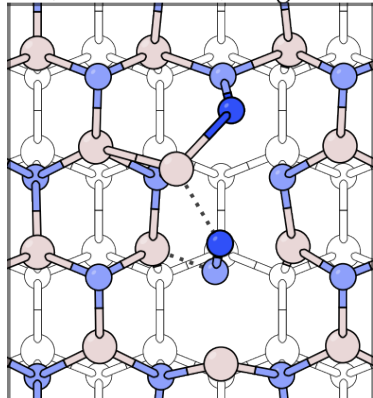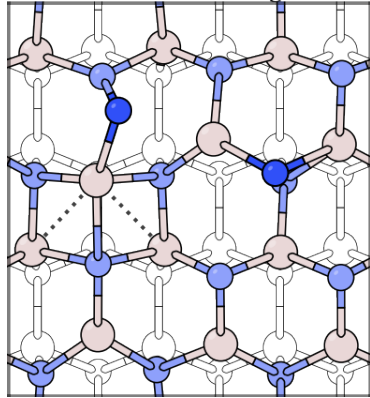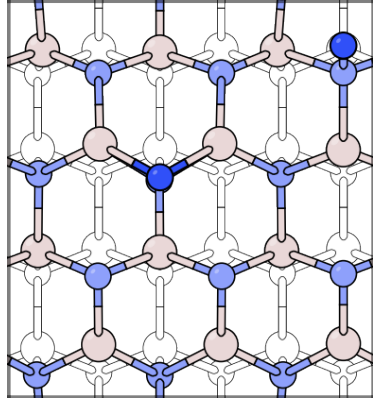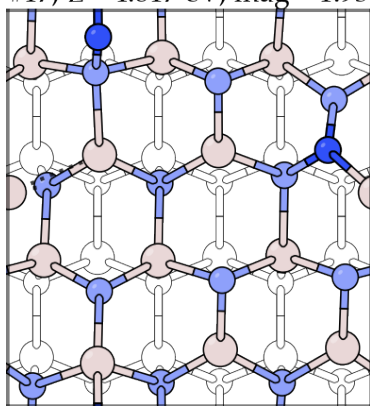
#13, E = 3.947 eV, mag = -0.00　　#14, E = 4.156 eV, mag = 2.00　　#15, E = 4.305 eV, mag = 2.00　　#16, E = 4.396 eV, mag = 2.00
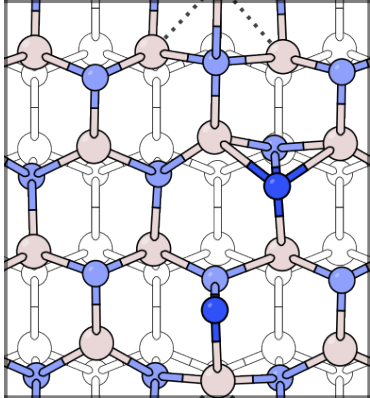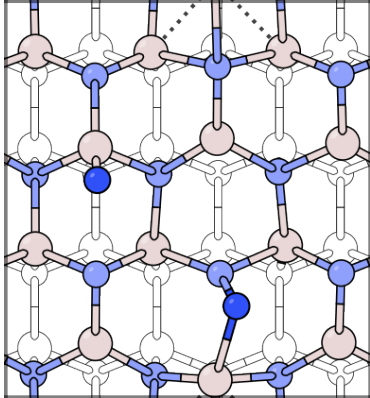
#17, E = 4.817 eV, mag = 1.93   #18, E = 4.953 eV, mag = 1.76