

Supplementary Material

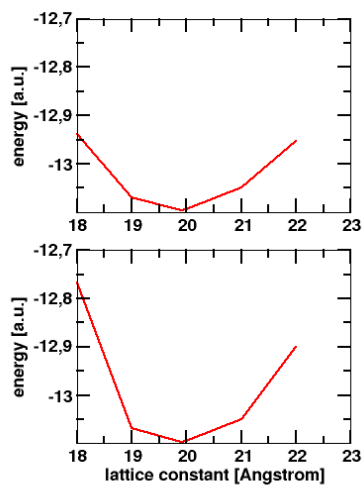


Figure S1: Cell constant depending on the plane-wave cutoff for the $3 \times 3 \times 3$ supercell. Upper graph: 50 Rydberg, lower graph: 70 Rydberg. Both graphs agree well with the experimental value of 19.90 a.u. ($3 \times 3.51 \text{ \AA}$, leading to a density of 0.534 g/cm^3 , <https://en.wikipedia.org/wiki/Lithium>, last accessed 16/06/2022).

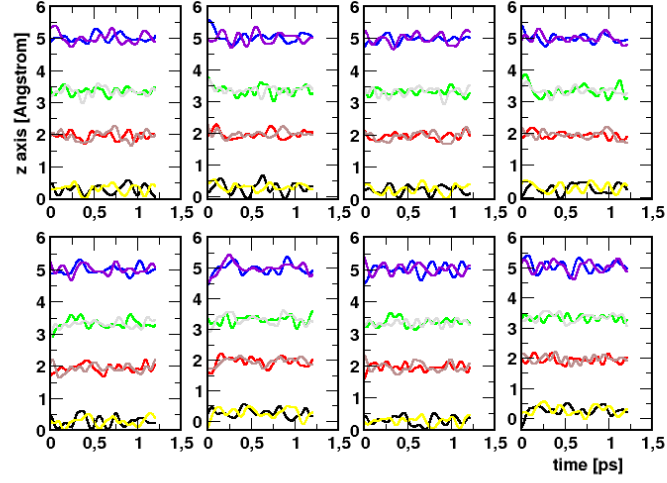


Figure S2: z-Axis of all the 64 lithium atoms in simulation **1**, eight atoms per plot (100 K). The structure is stable.

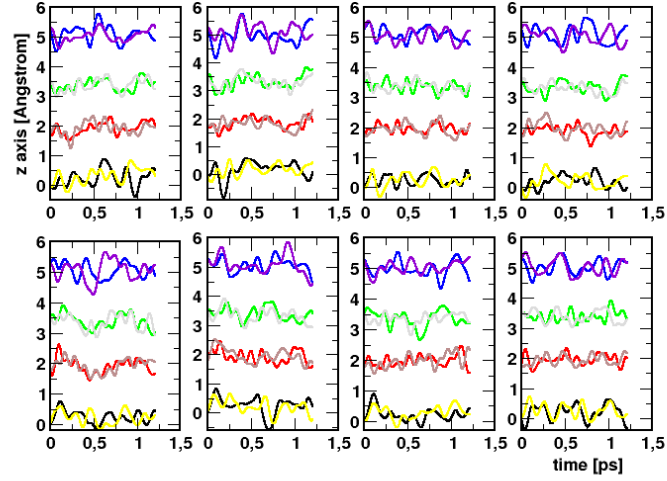


Figure S3: z-Axis of all the 64 lithium atoms in simulation **1**, eight atoms per plot (300 K). The structure is stable.

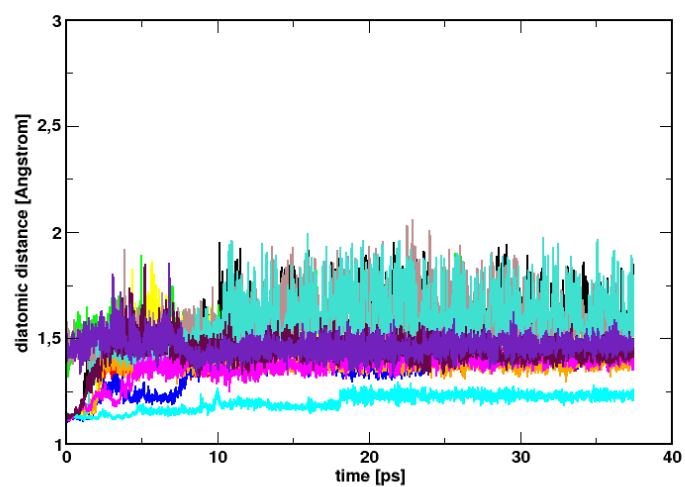


Figure S4: Diatomic distances of all nitrogen molecules in simulation **2** (300 K). The nitrogen molecules are integrated in the lithium slab which leads to an elongation of the nitrogen-nitrogen bond, but in this case to no bond breaking.

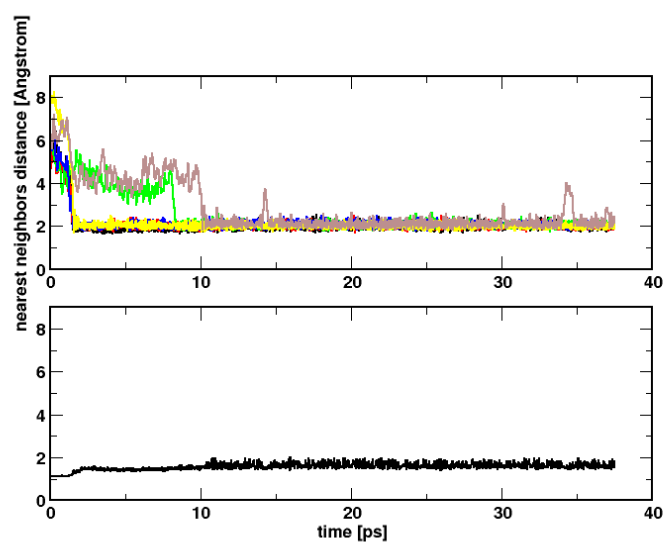


Figure S5: Simulation 2: Distances of the nearest neighbors, first nitrogen atom. Upper plot: lithium, lower plot: nitrogen. The nitrogen-nitrogen bond is weakened as the nitrogen molecule is integrated in the surface. In the end, it is surrounded by six lithium atoms.

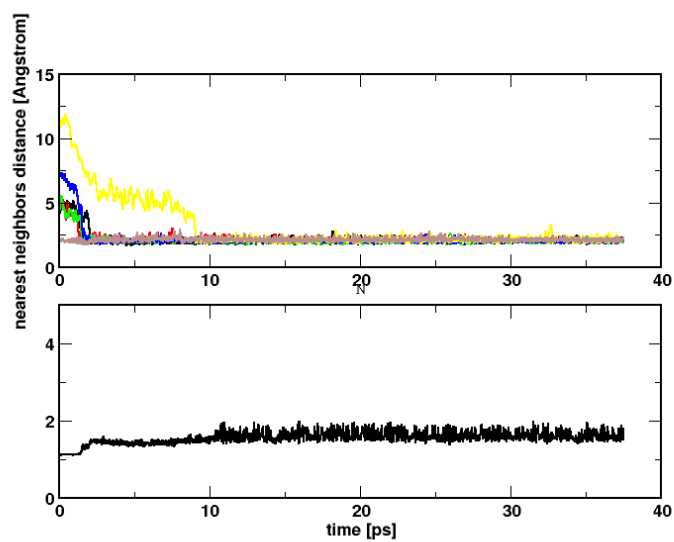


Figure S6: Simulation 2: Distances of the nearest neighbors, second nitrogen atom. Upper plot: lithium, lower plot: nitrogen. The nitrogen-nitrogen bond is weakened as the nitrogen molecule is integrated in the surface. In the end, it is surrounded by six lithium atoms.

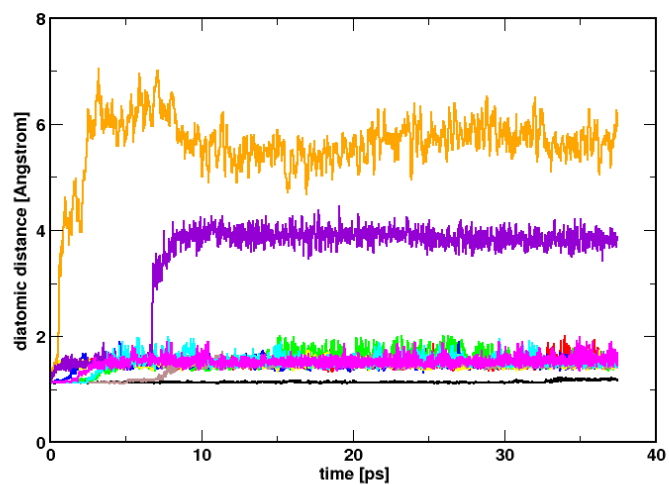


Figure S7: Diatomic distances of all nitrogen molecules in simulation **3** (300 K). Most nitrogen molecules are integrated in the lithium slab which leads to an elongation of the nitrogen-nitrogen bond. A single nitrogen molecule (black) remains unbound. Two nitrogen molecules (orange and lilac) dissociate.

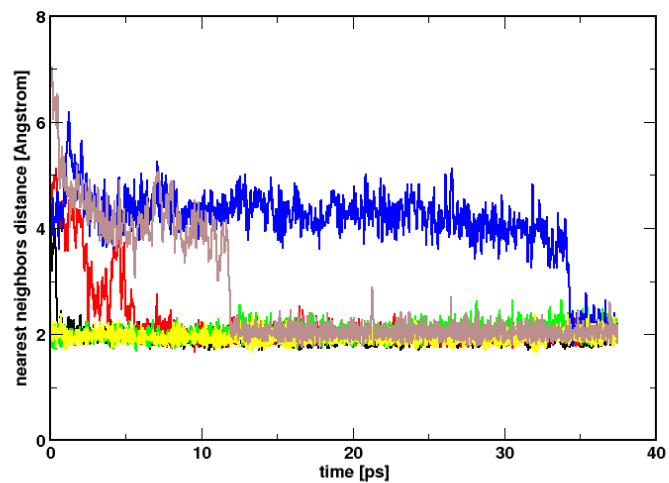


Figure S8: Simulation **3**: Distances of the nearest neighbors, first nitrogen atom. In the end, the nitrogen atom is surrounded by six lithium atoms.

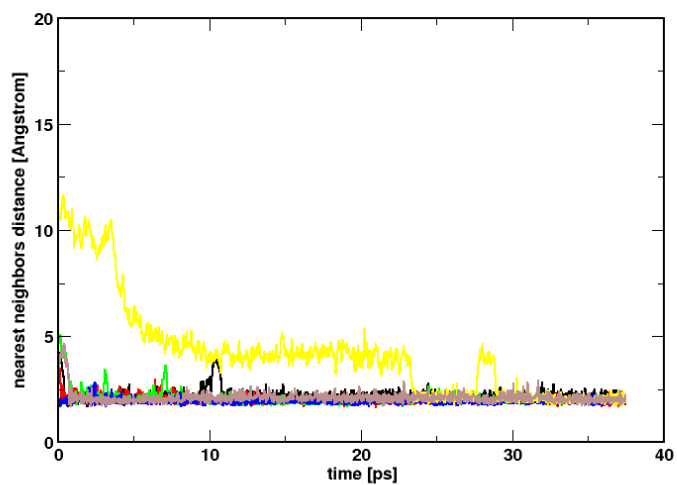


Figure S9: Simulation **3**: Distances of the nearest neighbors, second nitrogen atom. In the end, the nitrogen atom is surrounded by six lithium atoms.

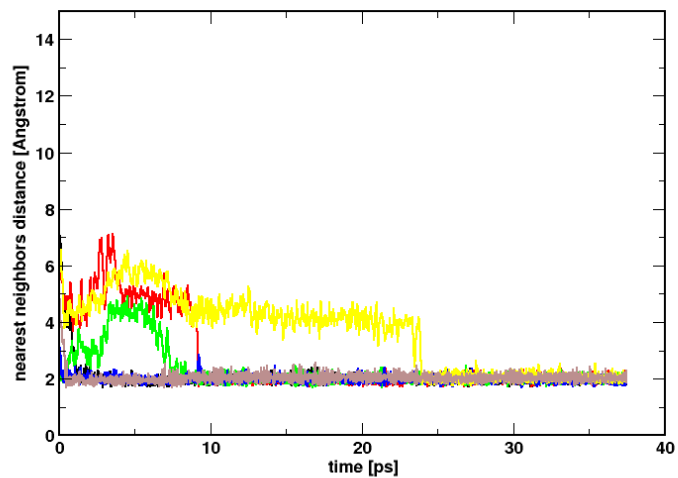


Figure S10: Simulation **3**: Distances of the nearest neighbors, third nitrogen atom. In the end, the nitrogen atom is surrounded by six lithium atoms.

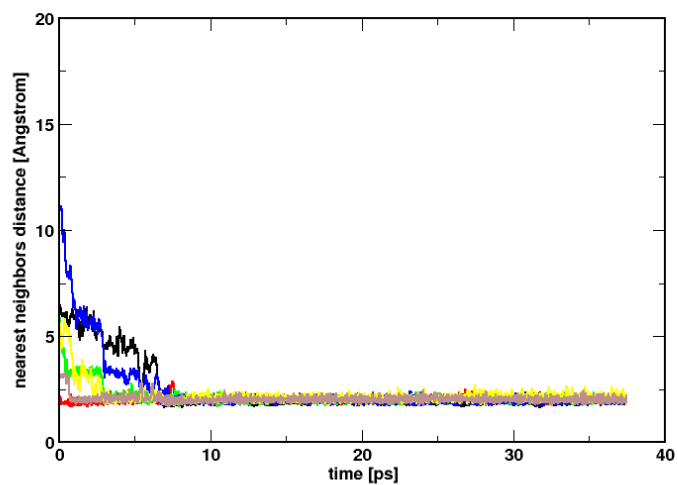


Figure S11: Simulation **3**: Distances of the nearest neighbors, fourth nitrogen atom. In the end, the nitrogen atom is surrounded by six lithium atoms.

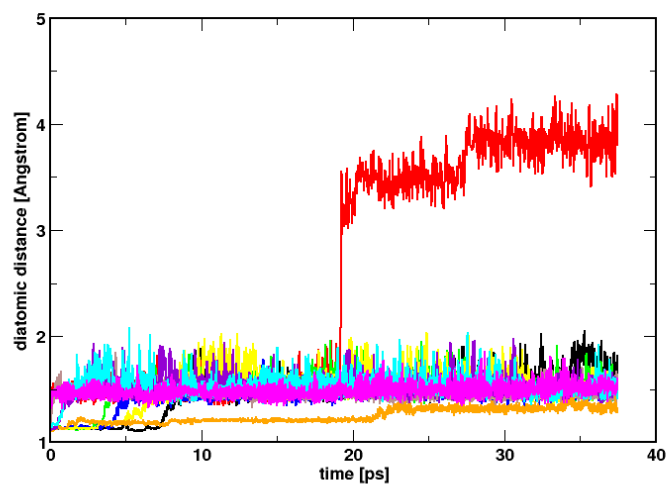


Figure S12: Diatomic distances of all nitrogen molecules in simulation 4 (300 K). A single nitrogen molecule dissociates.

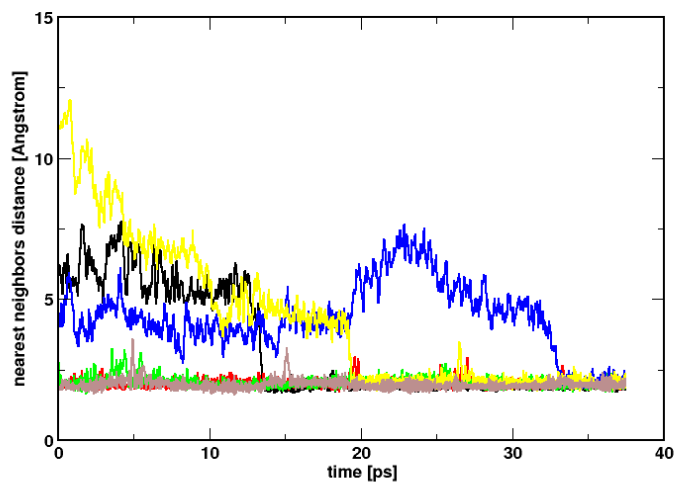


Figure S13: Simulation 4: Distances of the nearest neighbors, first nitrogen atom. In the end, the nitrogen atom is surrounded by six lithium atoms.

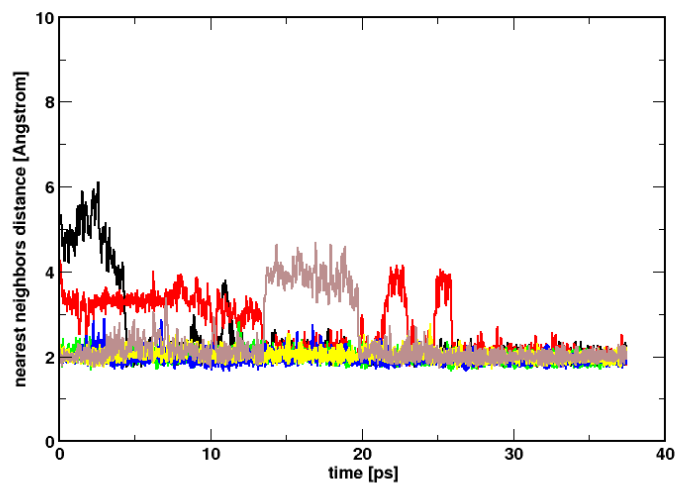


Figure S14: Simulation 4: Distances of the nearest neighbors, second nitrogen atom. In the end, the nitrogen atom is surrounded by six lithium atoms.

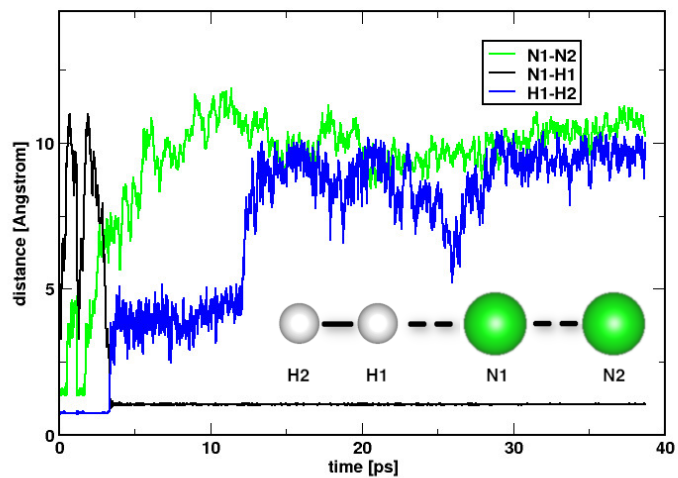


Figure S15: Simulation 11: Formation of the N-H bond, breaking of the N-N and H-H bonds.

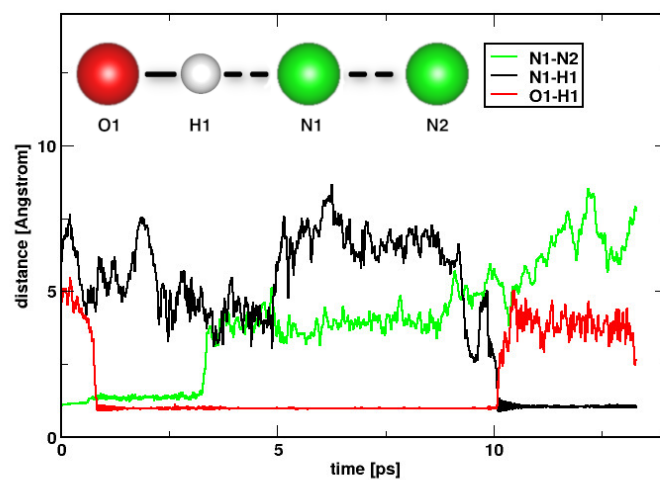


Figure S16: Simulation **20**: Formation of the N-H bond, breaking of the N-N and O-H bonds.

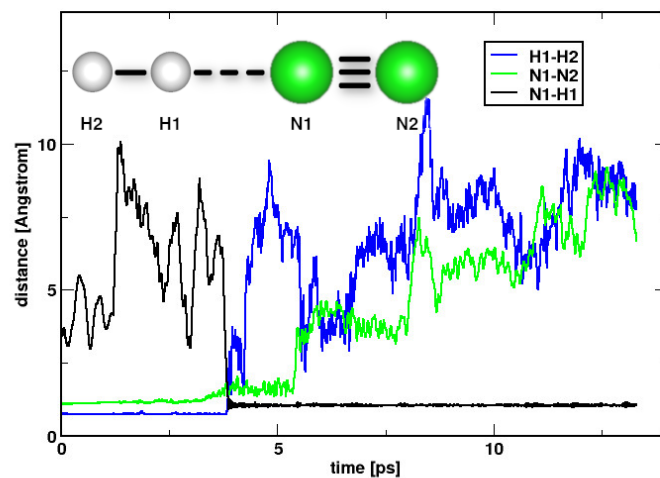


Figure S17: Simulation **24**: Formation of the N-H bond, breaking of the N-N and H-H bonds.