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Structures, stability, magnetic moments and growth strategies of the Fe_nN (n=1-7) clusters: all-electron density functional theory calculations

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Highlights:

- 1. The structural stability of the Fe_4N and Fe_6N clusters is higher.
- 2. The chemical stability of the Fe_3N and Fe_7N clusters is higher.
- 3. Fe_5 clusters are easier to adsorb a Fe atom while Fe_4 clusters are easier to adsorb a N atom.
- 4. Fe_nN clusters prefer to adsorb a Fe atom.

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