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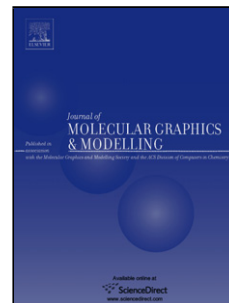
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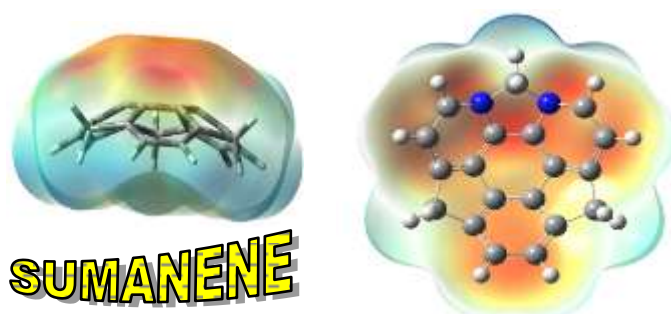
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Graphical abstract



Highlights

- Position of nitrogen atoms in frame of sumanene affects on interaction energies.
- Isomers are'nt perturbed significantly after adsorption so process is physisorption.
- ZPE and BSSE-corrected interaction energies were calculated for 26 sumanene isomers.
- Hub-hub and bridge-bridge categories are the best and the worst classes of isomers.

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