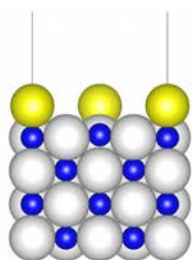


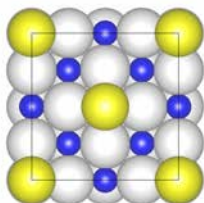
Supplementary Materials for:
**A rational computational study of surface defect-mediated
stabilization of low-dimensional Pt nanostructures on TiN(100)**

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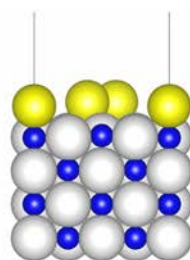
(Dated: February 4, 2015)



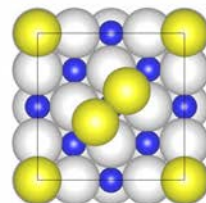
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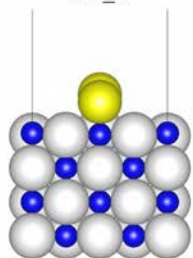
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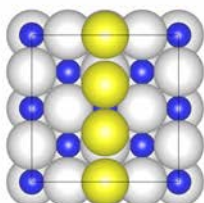
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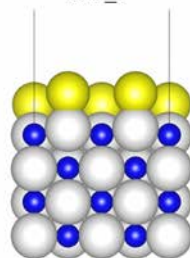
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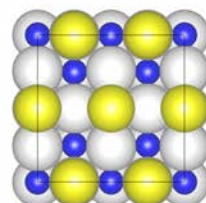
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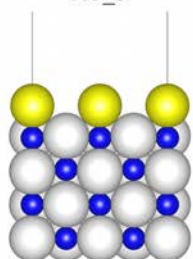
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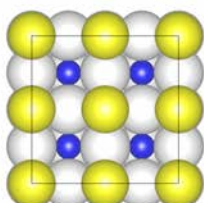
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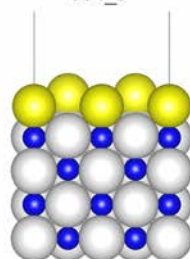
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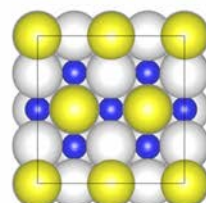
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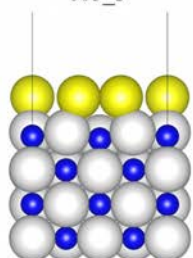
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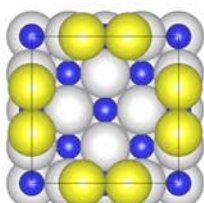
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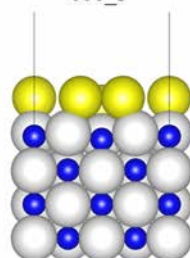
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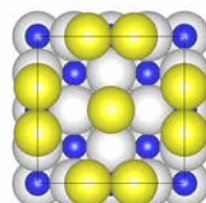
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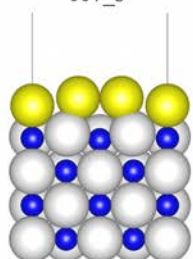
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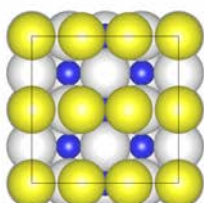
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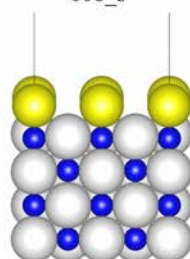
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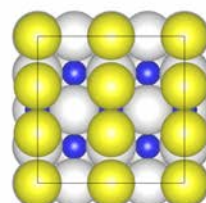
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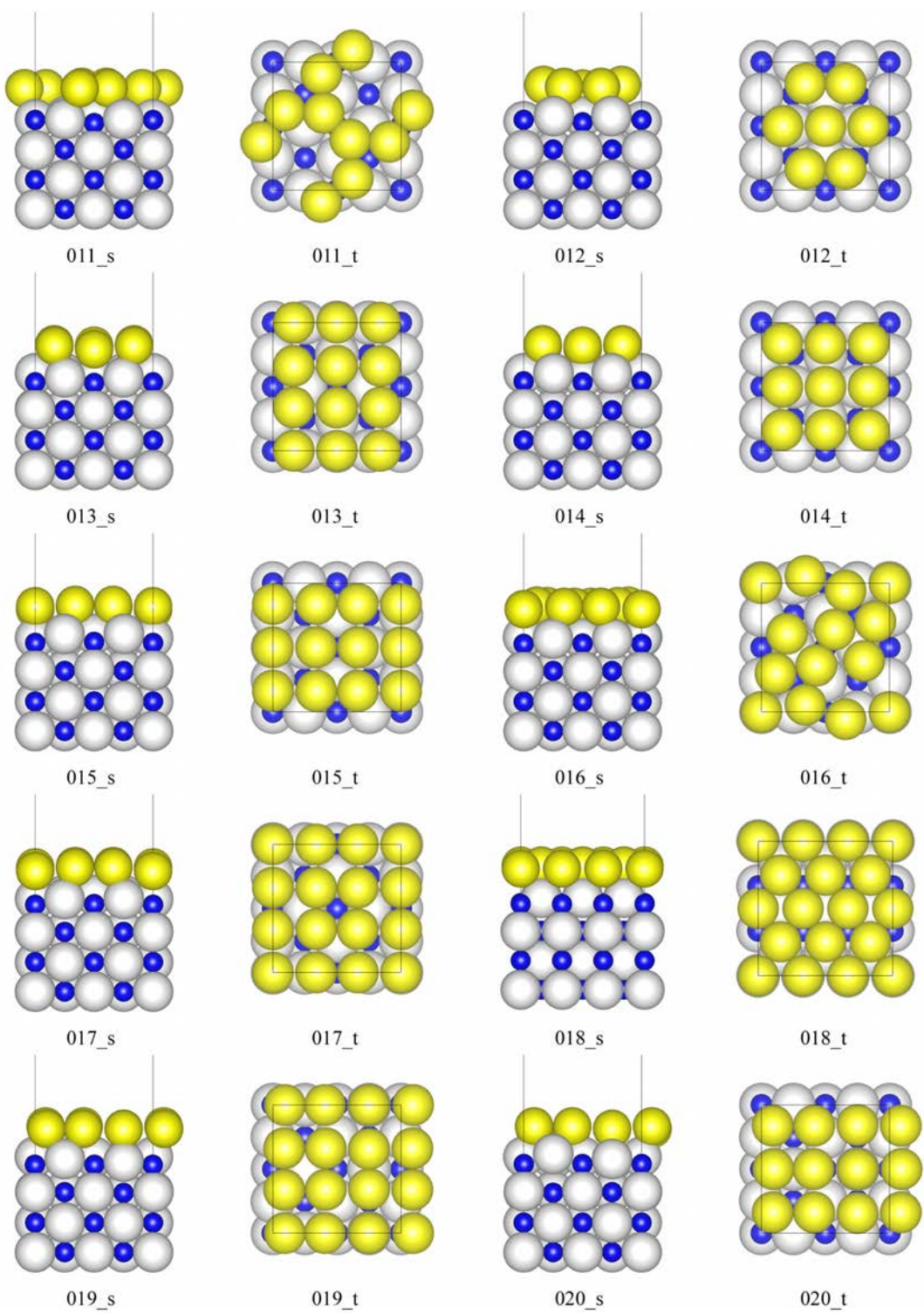
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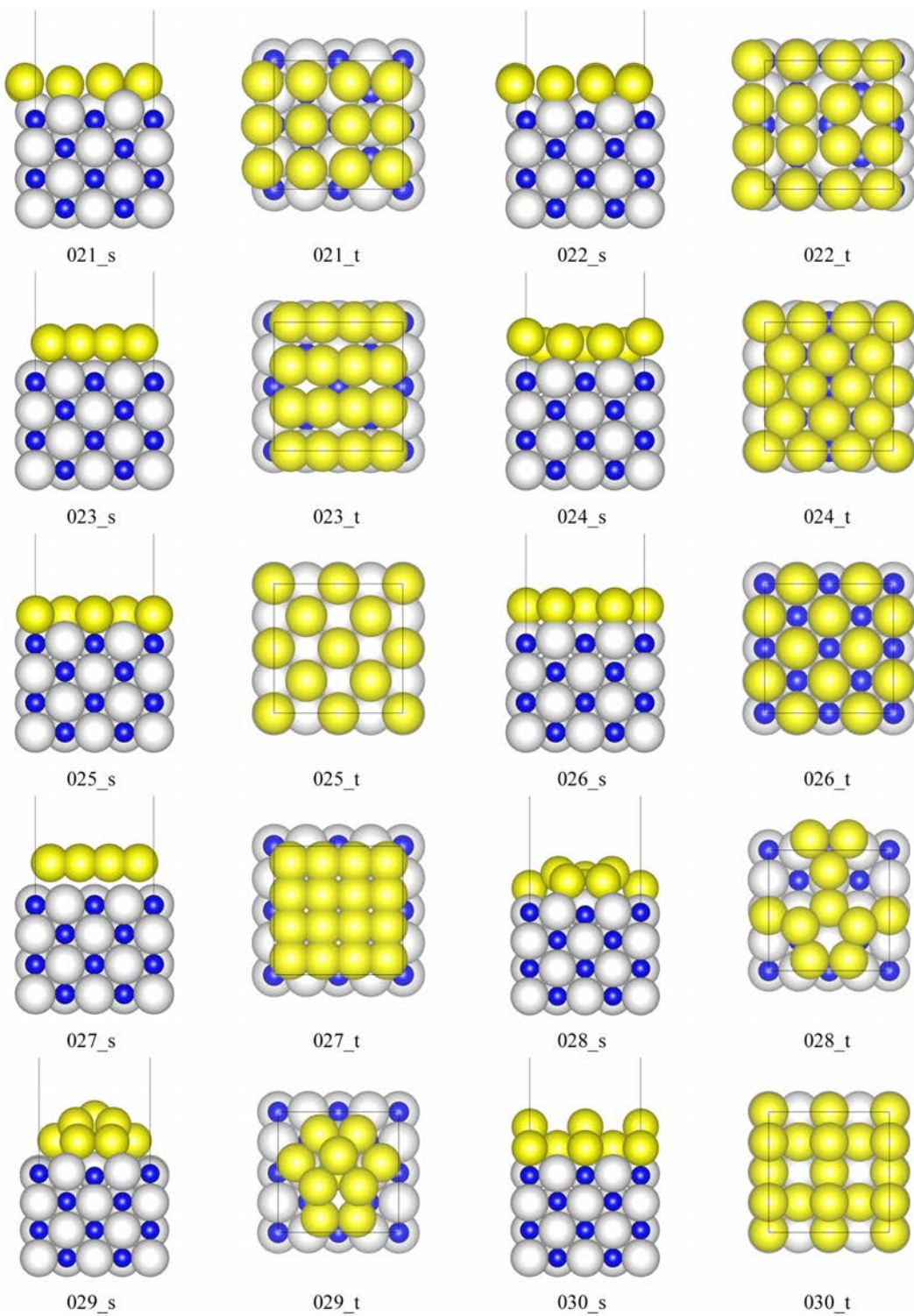


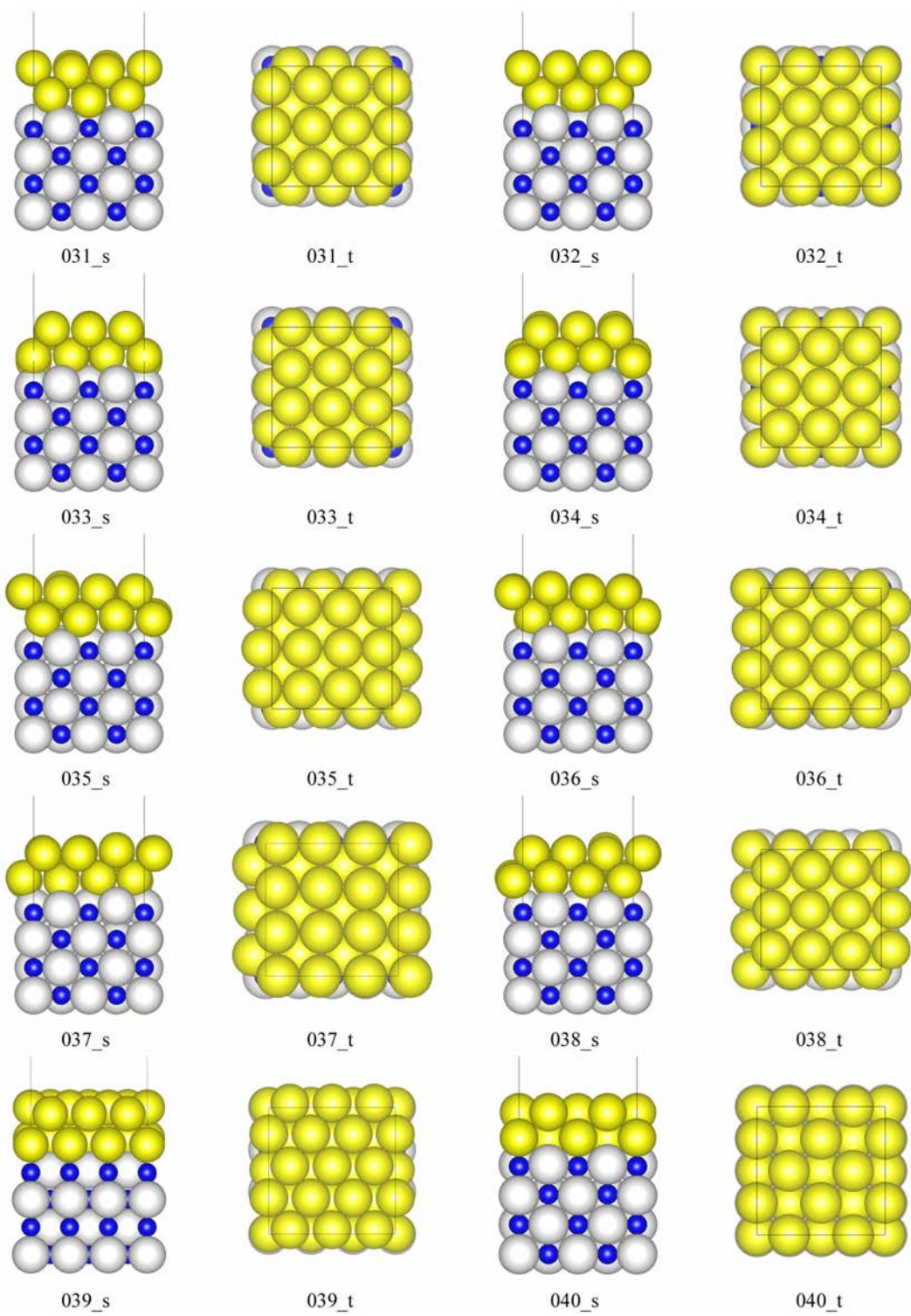
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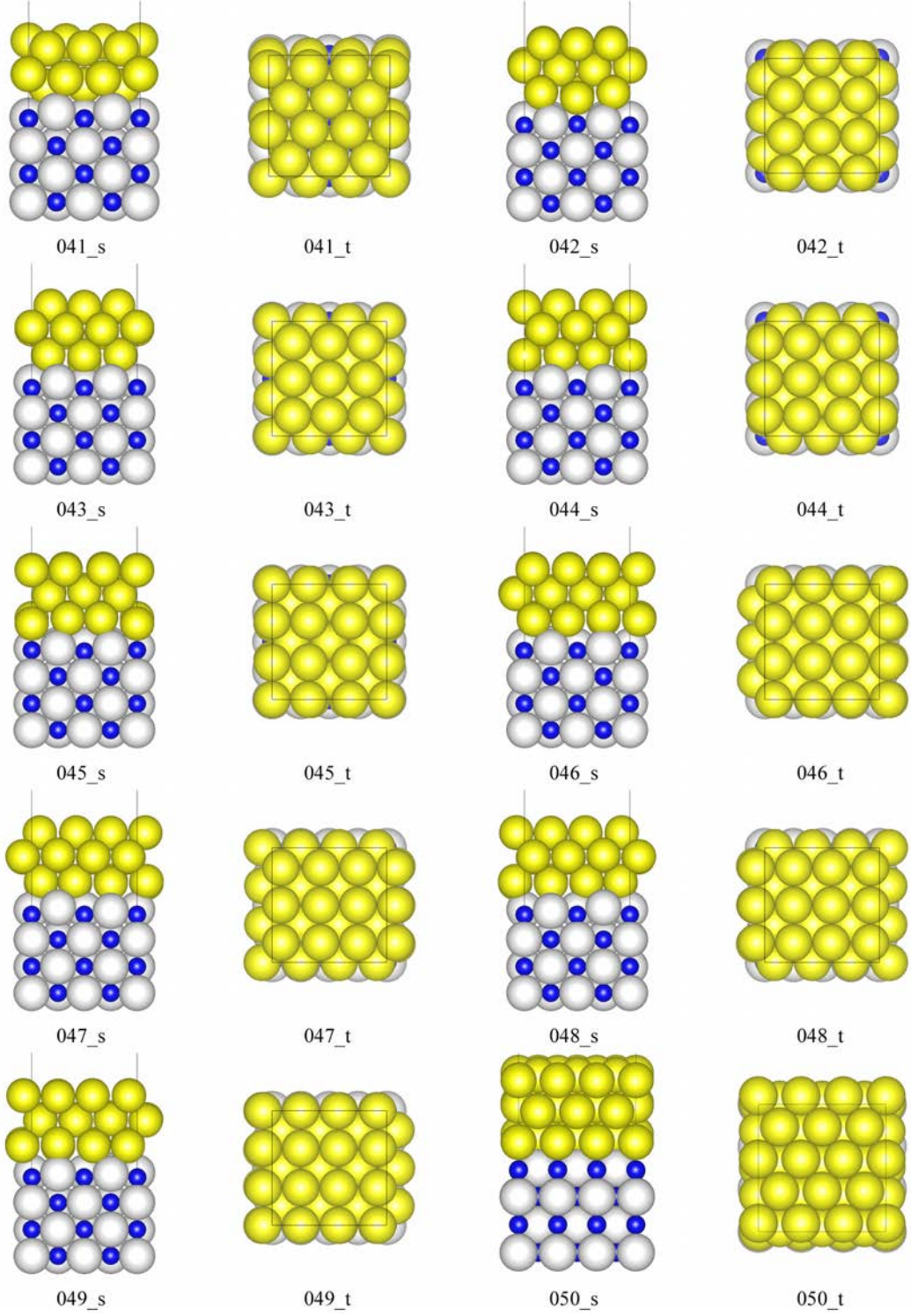


FIG. 1. Side- and top-view of the atomic structures of Pt nanostructures on pristine TiN(100) in a $p(3 \times 3)$ surface cell. These structures are labelled from 001 to 050 and the suffix “s” and “t” are used to differentiate the side- and top-views of a particular structure, accordingly. Here, the yellow, blue, and white spheres denote the Pt, N, and Ti atoms, respectively.

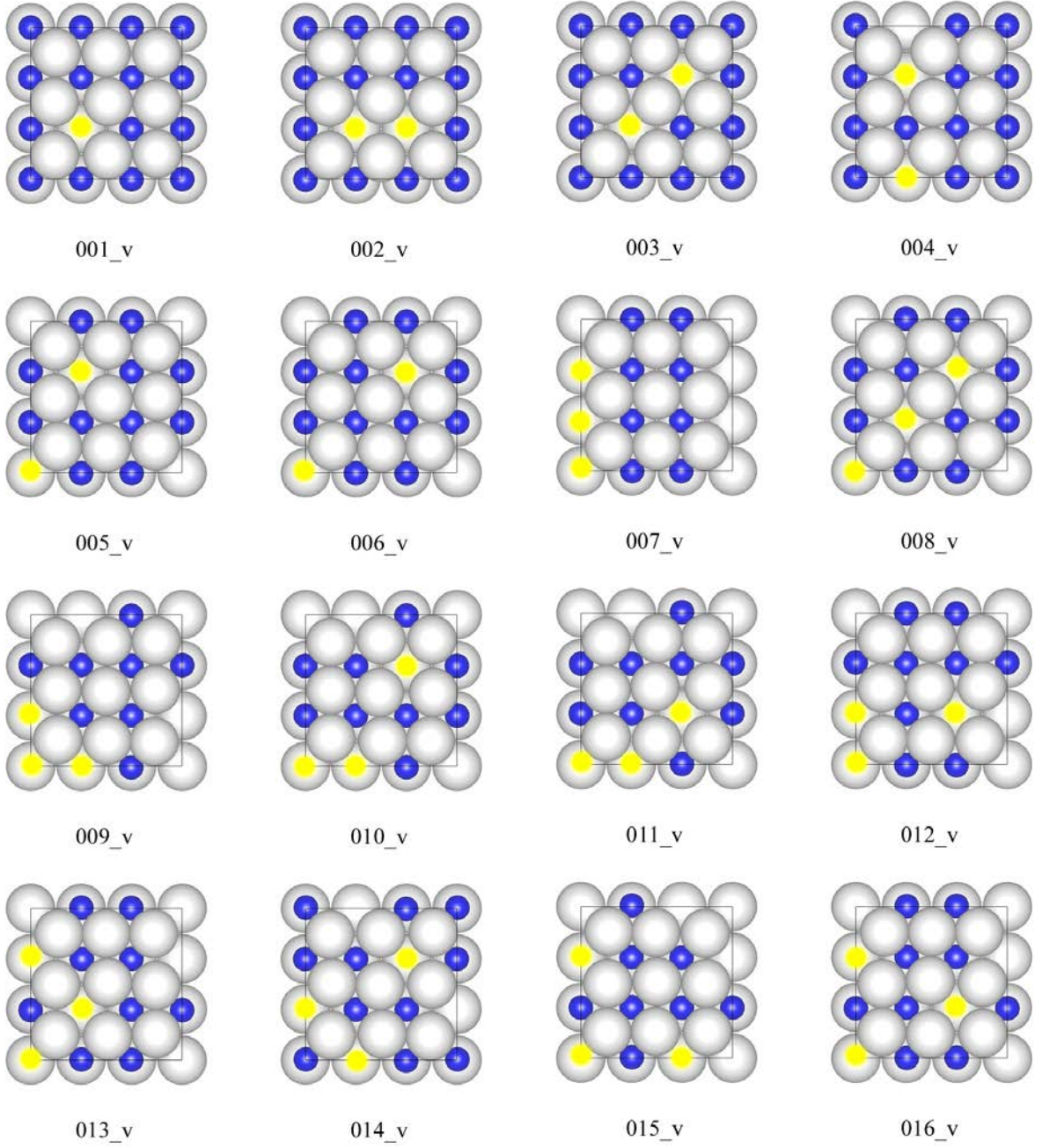


FIG. 2. Top-view of the atomic structures of the possible arrangements of surface nitrogen vacancies on TiN(100) in a $p(3 \times 3)$ surface cell. The structures labelled 001 contains one surface nitrogen vacancy, while 002 to 006 contain two surface nitrogen vacancies, and 007 to 016 three surface nitrogen vacancies, respectively. Here, the blue and white spheres denote the N and Ti atoms.

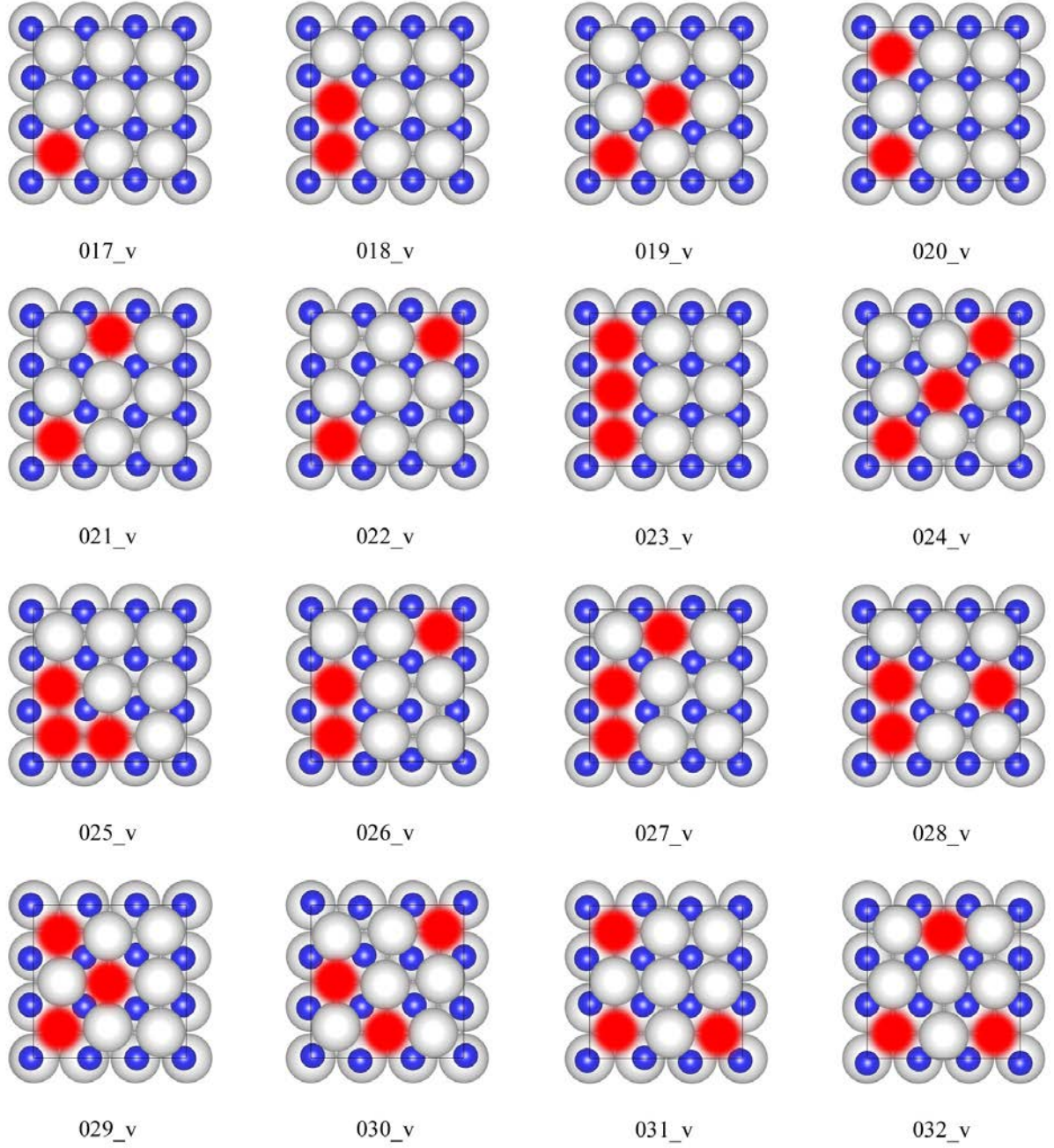


FIG. 3. Top-view of the atomic structures of the possible arrangements of surface titanium vacancies on TiN(100) in a $p(3 \times 3)$ surface cell. The structures labelled 017 contains one surface titanium vacancy, while 018 to 022 contain two surface titanium vacancies, and 023 to 032 three surface titanium vacancies, respectively. Here, the blue and white spheres denote the N and Ti atoms.