NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

SCBE21014- Engineering Coking-Resistant Catalysts in the Dry Reforming of Methane

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Background & Significance

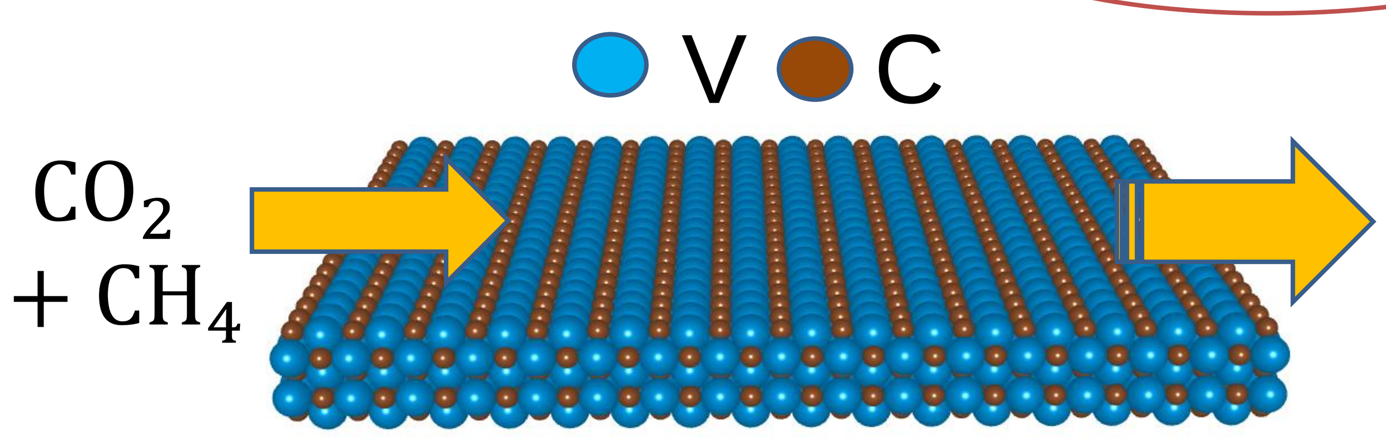
Methane Dry Reforming

- ↓ Greenhouse Emissions
- Environmental Protection
- ↑ Syngas Production

Singapore Carbon Industry

- Achieve net-zero emissions by 2050 [2]
- Focus on H_2 production & CO_2 utilisation [2]

$$CO_2 + CH_4 \leftrightarrow \boxed{2H_2 + 2CO}$$



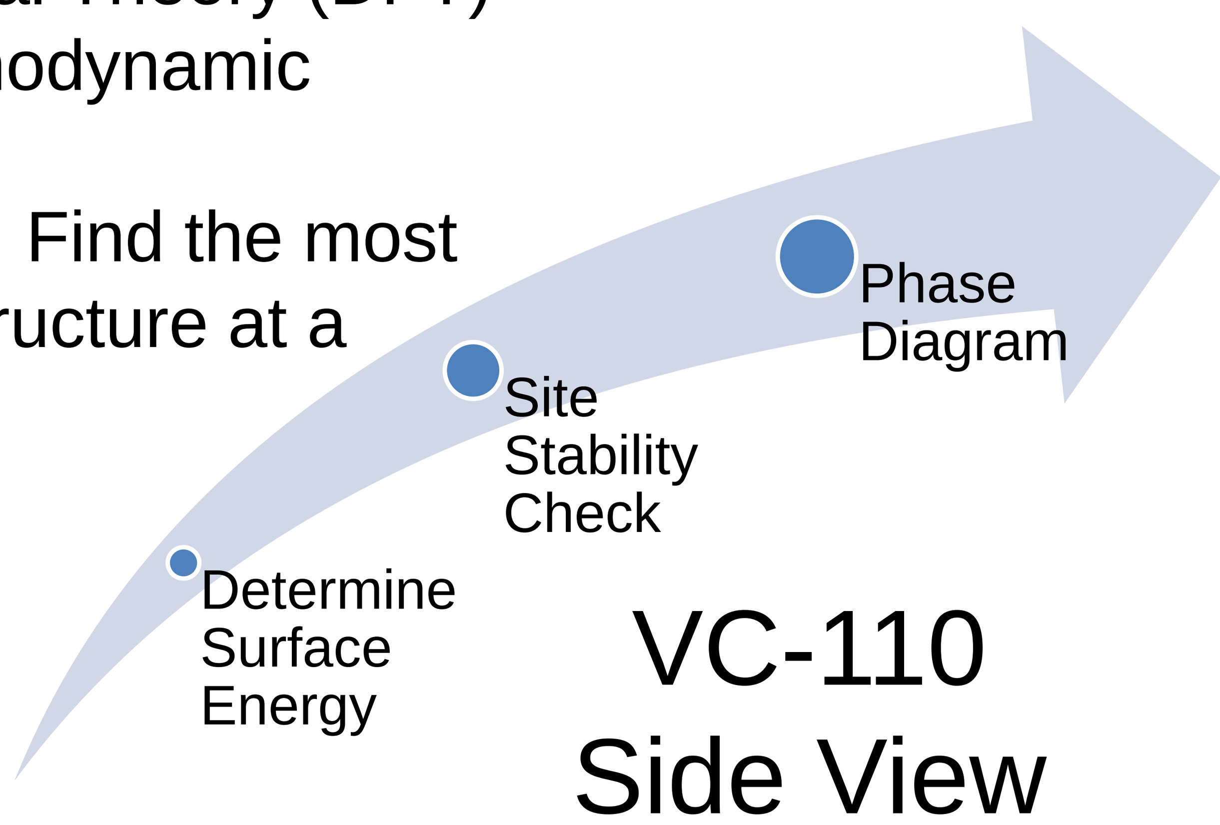
Syngas – key intermediate for the chemical industry

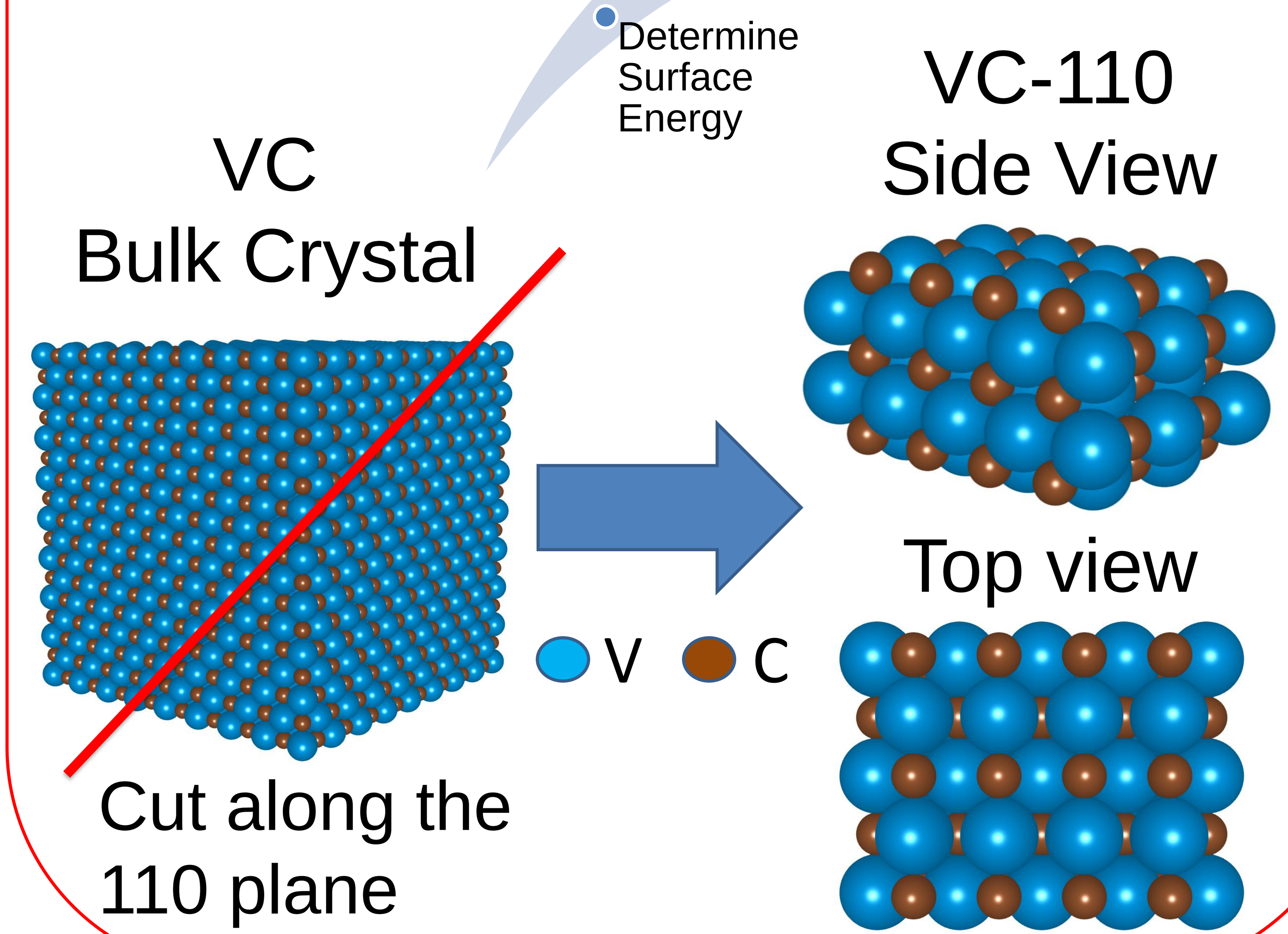
Current Roadblocks:

- Earth-abundant metal catalysts (Pt, Ni, Vanadium Carbide (VC)) are inefficient (coking/sintering) [1]
- Limited Breakthroughs with current technology

Computational Modelling

- Density Functional Theory (DFT) paired with thermodynamic calculations
- Phase Diagrams: Find the most stable catalyst structure at a desired P and T

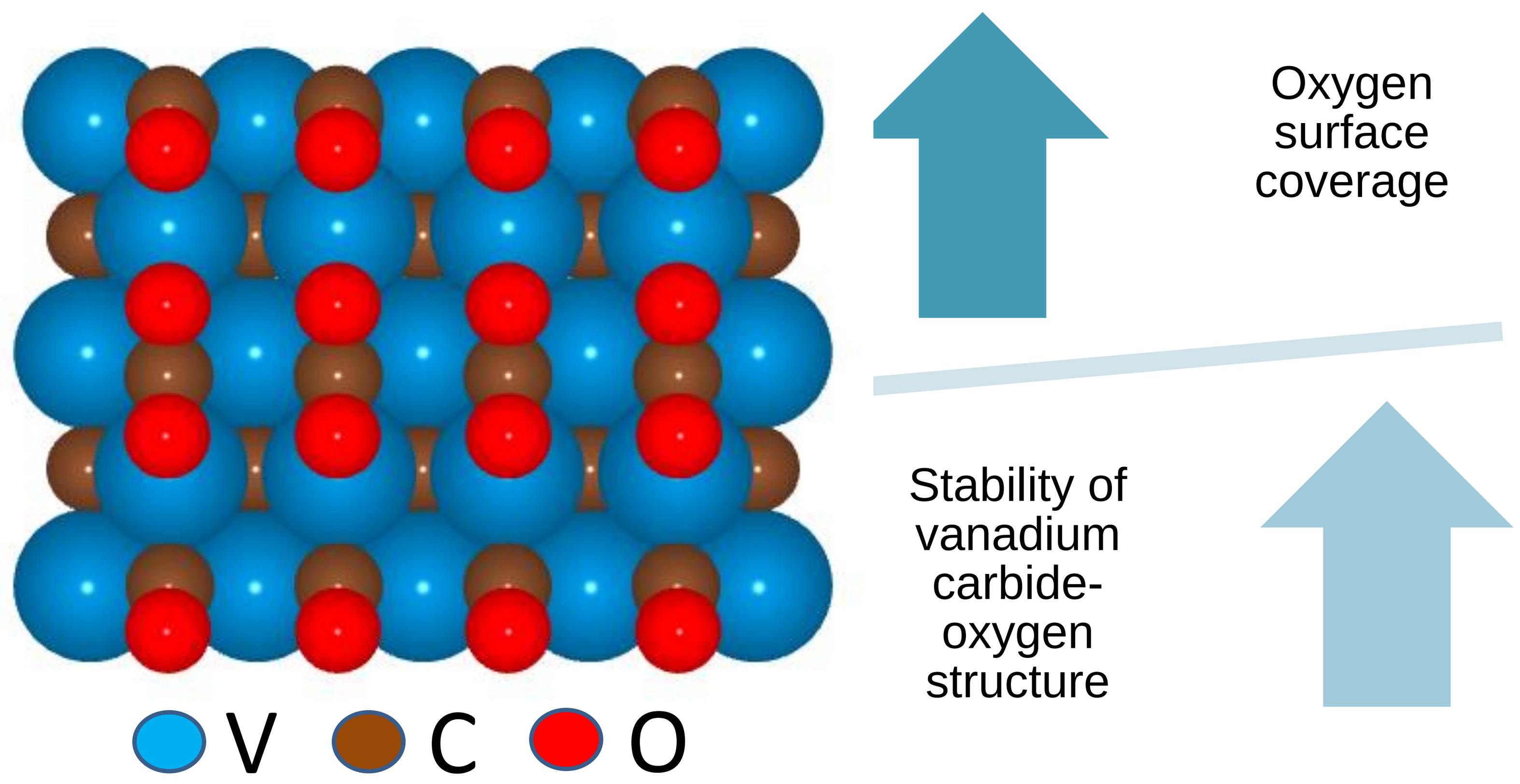


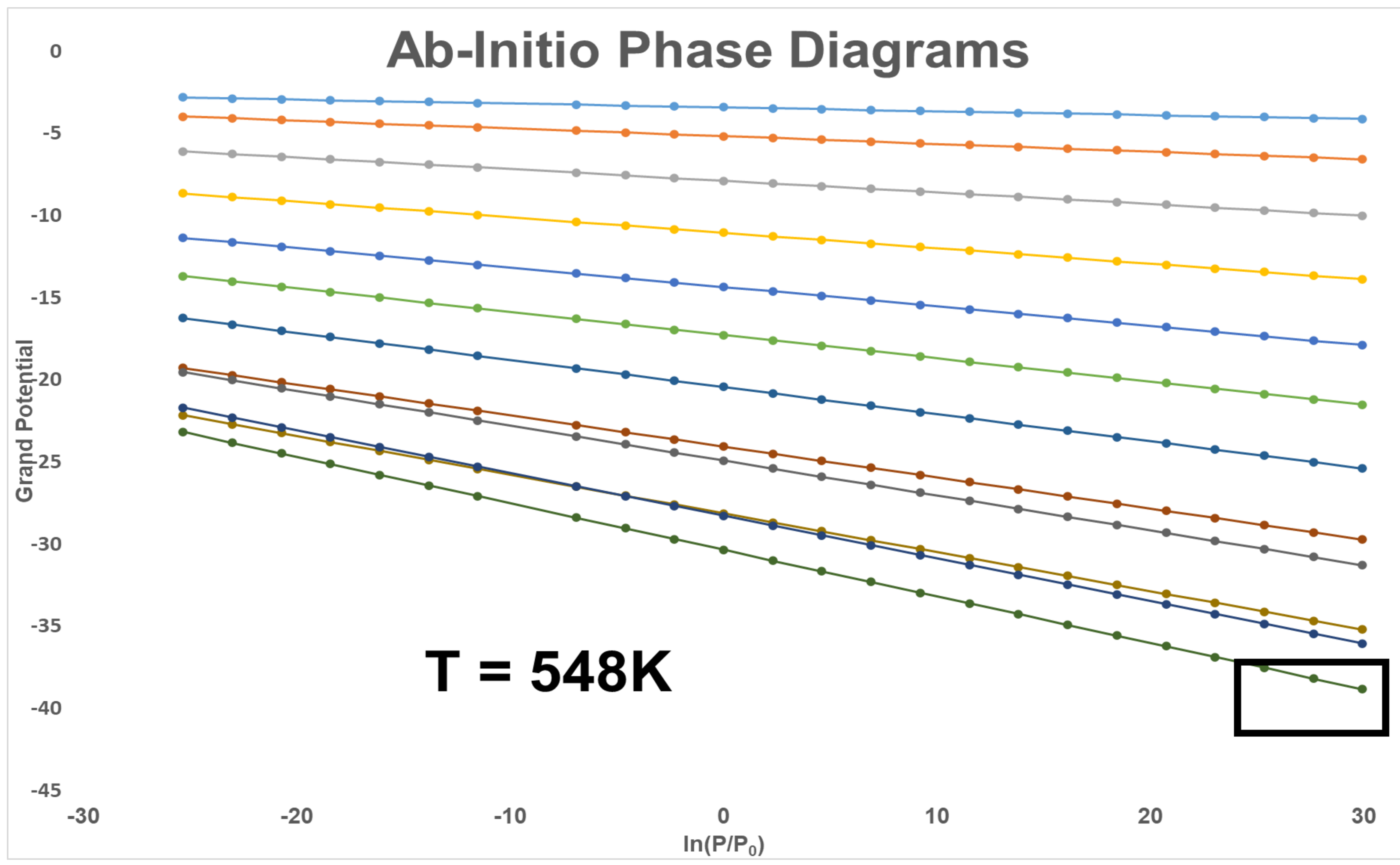


Cut along the 110 plane

Results & Discussion

- V-C-bridge site is most stable; Most stable structure achieved by adding 12 oxygens on the surface.





Total of 12 Phase Diagrams

Conclusion & Future Work

- Improve phase diagram accuracy by adding more surface oxygen arrangements.
- Explore adding oxygen atoms to other locally stable adsorption sites found (V-top site).
- Extend current work to include oxy-carbides, which are experimentally coke-resistant.

References

- [1] X. Gao, J. Ashok and S. Kawi, “Smart Designs of Anti-Coking and Anti-Sintering Ni-Based Catalysts for Dry Reforming of Methane: A Recent Review”, 2020.
- [2] H. C. Lau, S. Ramakrishna, K. Zhang and Mohamed Z. S. Hameed, “A Decarbonization Roadmap for Singapore and Its Energy Policy Implications, 2021.

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