## Nature Friendly Single Atom Pt Catalyst For Propane Dehydrogenation

## **Supporting Information**

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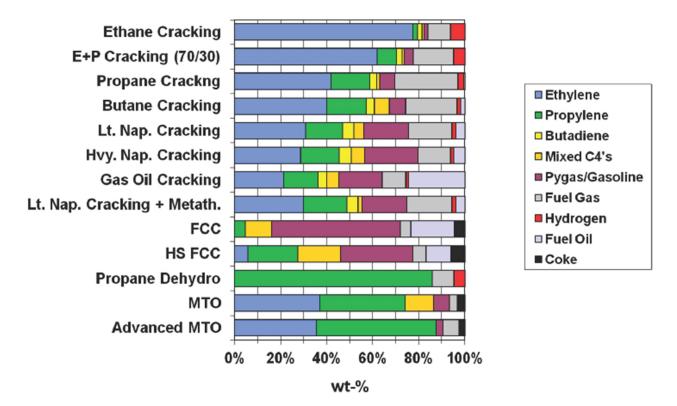


Figure S1- Weigh percent production rate Of Propylene from different methods in 2016 [1].

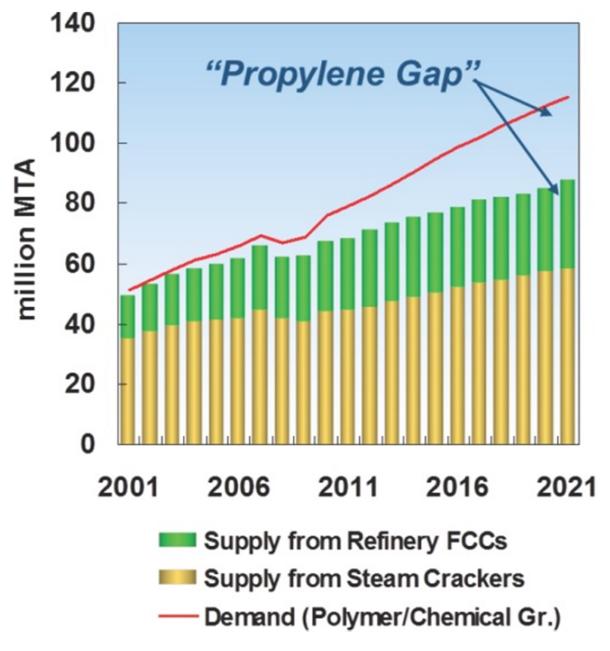


Figure S2- Predicted demand of propylene up to 2021 [1].

Mechanism 1:  $C_3H_8(g)+S{\leftrightarrow}C_3H_8$ ...S  $C_3H_8{}^{\cdots}S{+}S{\longleftrightarrow}C_3H_7{}^{\cdots}S{+}H{}^{\cdots}S$ Rate Determinig Step  $C_3H_7^{\cdots}S+S{\longleftrightarrow}C_3H_6^{\cdots}S+H^{\cdots}S$  $C_3H_6$   $\longrightarrow$   $C_3H_6(g)+S$ 2H<sup>...</sup> $S \leftrightarrow H_2(g) + 2S$  $CH_4 \!\!+\!\! S \!\!\leftrightarrow\!\! CH_4 \!\!\cdots\!\! S$  $C_2H_4 \!\!+\!\! S \!\!\leftrightarrow\!\! C_2H_4 \!\!\cdots\!\! S$  $C_2H_6+S \leftrightarrow C_2H_6$  "S Mechanism 2:  $C_3H_8(g) + 2S {\longleftrightarrow} C_3H_7 {^{\cdots}S} + H {^{\cdots}S}$ Rate Determinig Step  $C_3H_7^{\cdots}S+S{\leftrightarrow}C_3H_6^{\cdots}S+H^{\cdots}S$  $C_3H_6$   $\cdots$   $S \leftrightarrow C_3H_6(g) + S$  $2H^{\cdots}S \leftrightarrow H_2(g)+2S$  $CH_4 \!\!+\!\! S \!\!\leftrightarrow\!\! CH_4 \!\!^{\dots} \! S$  $C_2H_4 \!\!+\!\! S \!\!\leftrightarrow\!\! C_2H_4 \!\!\cdots\!\! S$  $C_2H_6+S \leftrightarrow C_2H_6$ ...S Mechanism 3:  $C_3H_8(g)+S \leftrightarrow C_3H_7$  ··· S ··· H Rate Determinig Step  $C_3H_7^{\cdots}S^{\cdots}H{\leftrightarrow}C_3H_6^{\cdots}S^{\cdots}H{+}H^{\cdots}S$  $C_3H_6{}^{\cdots}S{}^{\cdots}H{\leftrightarrow}C_3H_6(g){+}H{}^{\cdots}S$  $2H^{\cdots}S \leftrightarrow H_2(g)+2S$  $CH_4+S \leftrightarrow CH_4$ ...S  $C_2H_4+S \leftrightarrow C_2H_4$ ...S  $C_2H_6 + S {\longleftrightarrow} C_2H_6 {\overset{\dots}{-}} S$ Mechanism 4:  $C_3H_8(g)+S \leftrightarrow C_3H_7$  "S"H Rate Determinig Step  $C_3H_7$ ···S···H $\leftrightarrow$  $C_3H_6(g)+H$ ···S···H  $H^{\cdots}S^{\cdots}H \leftrightarrow H_2(g)+S$  $CH_4 \!\!+\!\! S \!\!\leftrightarrow\!\! CH_4 \!\!^{\dots} \! S$  $C_2H_4 + S {\longleftrightarrow} C_2H_4 {\overset{\dots}{}} S$  $C_2H_6+S\leftrightarrow C_2H_6$ ...S

Scheme S1- Four most accepted Langmuire-Hinshelwood mechanisms of propane dehydrogenation [2].

## References:

- 1. Bell AT, Alger MM, Flytzani-Stephanopoulos M, Gunnoe TB, Lercher JA, Stevens J, Alper J, Tran C (2016) The Changing Landscape of Hydrocarbon Feedstocks for Chemical Production: Implications for Catalysis. In: National Academies of Sciences, Engineering, and Medicine, Washington, DC, USA.
- 2. Fogler H (1999) Elements of chemical reaction engineering, 3rd. In.: Prentice Hall International, Inc, New Jersey.