Chemistry with Computers

Yingbin Ge

Si nanoclusters emit bright light

Bulk silicon

EXCEL calculated energy of H₂

Transition Metal Catalyst

C₃H₈ + 1/2O₂ → C₃H₆ + H₂O

Energy surfaces of two-dimensional H₂

Energy (au)

Bond distance (au)

EXCEL calculated energy of H₂

Spreadsheet

HF/STO-3G

HF/cc-pV6Z

C₃H₈ + 1/2O₂ → C₃H₆ + H₂O
Recent publications

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