

## SUPPORTING INFORMATION

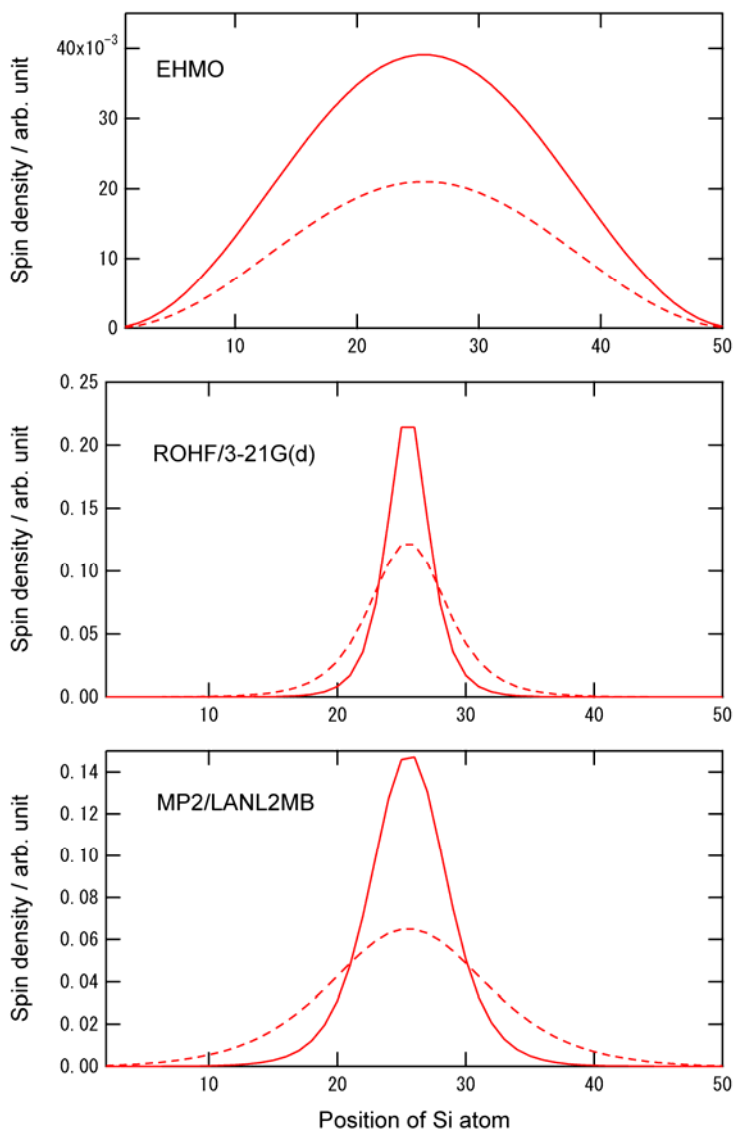
### Mechanism of Electron and Hole Localization in Poly(dimethylsilane) radical ions

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#### 1. Spin density distributions calculated by means of EHMO, ROHF and MP2 methods



*Figure S1.* Spin densities of the hole and excess electron in  $\text{CH}_3(\text{Si}(\text{CH}_3)_2)_n\text{CH}_3$  ( $n=50$ ) calculated by means of extended Huckel MO (EHMO), ROHF/3-21G(d) and MP2/LANL2MB methods. Solid and dashed lines indicate spin densities of cation and anion radicals, respectively.

## 2. Spin density distributions calculated by means of DFT (B3LYP and PW91PW91) methods

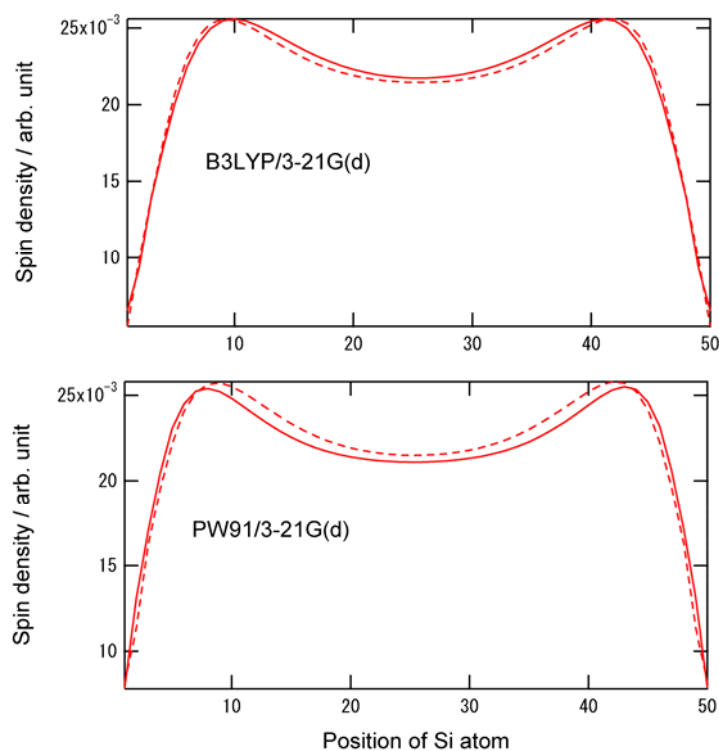


Figure S2. Spin densities of the hole and excess electron in  $\text{CH}_3(\text{Si}(\text{CH}_3)_2)_n\text{CH}_3$  ( $n=50$ ) calculated by means of B3LYP and PW91 methods. Solid and dashed lines indicate spin densities of cation and anion radicals, respectively.