

## MATTERS ARISING


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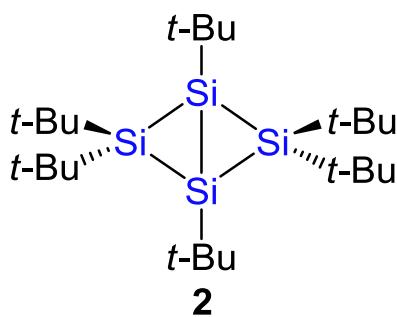
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# Reply to: “A double bond with weak $\sigma$ - and strong $\pi$ -interactions is still a double bond”

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REPLYING TO C. Foroutan-Nejad *Nature Communications* <https://doi.org/10.1038/s41467-021-24238-x> (2021)

In our original paper<sup>1</sup>, we reported synthesis of 1,2,2,3,4,4-hexa-*tert*-butylbicyclo[1.1.0]tetrasilane (**2**, Fig. 1). The X-ray crystallography of **2** showed a planar geometry around the bridgehead silicon atom (angle sums except for the inter-bridgehead bond = 359.79°). On the basis of experimental results of X-ray crystallography, electron paramagnetic resonance, magnetic susceptibility, UV/Vis and <sup>29</sup>Si NMR spectra, and theoretical calculations including natural bond orbital analysis, we concluded that **2** has a silicon–silicon  $\pi$  single bond between the bridgehead silicon atoms. We have been aware that the HOMO-6 and HOMO-1 represent in-phase and out-of-phase orbital interactions between the linearly arranged two  $\sigma$ (Si<sub>bridgehead</sub>–C<sub>tert</sub>-butyl) orbitals, respectively. We did not discuss them in the original paper because (i) we considered that the  $\sigma$ -type bonding interaction between the bridgehead silicon atoms due to the in-phase interaction (HOMO-6) should be canceled out by the corresponding out-of-phase interaction (HOMO-1) and (ii) we did not find  $\sigma$ -type interaction between the bridgehead silicon atoms within the above-mentioned our theoretical investigation (output threshold > 2.1 kJ mol<sup>-1</sup>).



**Fig. 1** Chemical structure of **2**.

In their commentary, Dr. Foroutan-Nejad took a different approach to characterize **2**. The author analyzed electron density of **2** theoretically and concluded that the silicon–silicon  $\pi$  bond is accompanied by a weak but non-negligible  $\sigma$  bond. We welcome discussion about the unusual bonding situation in the isolable compound **2** from diverse viewpoints to obtain deeper understanding of this chemical bond.

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## Reference

1. Kyushin, S. et al. Silicon–silicon  $\pi$  single bond. *Nat. Commun.* **11**, 4009 (2020).

## Author contributions

S.K., S.I. and H.M. discussed the content of this reply and wrote the manuscript. Y.K., K.O., H.I., T.K. and M.H. read and agreed to this reply.

## Competing interests

The authors declare no competing interests.

## Additional information

Correspondence and requests for materials should be addressed to S.K., S.I. or H.M.

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