



## Correction to: On fractional charge in molecules and materials

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### Correction to:

**Theoretical Chemistry Accounts (2020) 139:84**

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In the original publication of the article, in the Appendix section, under the heading “Calculations by density functional theory-based methods” the ionization potential (IP) equation incorrectly appears as  $IP = IP = E_{M^+} - E_M$ .

The correct equation is as below:

$$IP = E_{M^+} - E_M$$

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The original article can be found online at <https://doi.org/10.1007/s00214-020-2580-5>.

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