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Corrigendum

On-site approximation for spin–orbit coupling in linear combination of atomic orbitals density functional methods

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We have been kindly informed of some minor errors in the above paper.

(1) On page 8003 equation (15) is not correct. The correct formulae (and the ones actually programmed) are as follows:

$$
\begin{aligned}
\langle l_i, M_i|L_z|l_i, M_j\rangle &= -\,iM_i\delta(M_i + M_j = 0)\\
\langle l, 0|L_\mp|l, M_j\rangle &= \pm\sqrt{\frac{l(l+1)}{2}}\delta(M_j = 1) - i\sqrt{\frac{l(l+1)}{2}}\delta(M_j = \bar{1})\\
\langle l, 1|L_\mp|l, M_j\rangle &= -\,i\frac{\sqrt{l(l+1)-2}}{2}\delta(M_j = \bar{2}) \mp \sqrt{\frac{l(l+1)}{2}}\delta(M_j = 0)\\
&\quad \pm \frac{\sqrt{l(l+1)-2}}{2}\delta(M_j = 2)\\
\langle l, \bar{1}|L_\mp|l, M_j\rangle &= \pm\frac{\sqrt{l(l+1)-2}}{2}\delta(M_j = \bar{2}) + i\sqrt{\frac{l(l+1)}{2}}\delta(M_j = 0)\\
&\quad + i\frac{\sqrt{l(l+1)-2}}{2}\delta(M_j = 2)\\
\langle l, 2|L_\mp|l, M_j\rangle &= -\,i\frac{\sqrt{l(l+1)-6}}{2}\delta(M_j = \bar{3}) - i\frac{\sqrt{l(l+1)-2}}{2}\delta(M_j = \bar{1})\\
&\quad \mp \frac{\sqrt{l(l+1)-2}}{2}\delta(M_j = 1) \pm \frac{\sqrt{l(l+1)-6}}{2}\delta(M_j = 3)\\
\langle l, \bar{2}|L_\mp|l, M_j\rangle &= \pm\frac{\sqrt{l(l+1)-6}}{2}\delta(M_j = \bar{3}) \mp \frac{\sqrt{l(l+1)-2}}{2}\delta(M_j = \bar{1})\\
&\quad + i\frac{\sqrt{l(l+1)-2}}{2}\delta(M_j = 1) + i\frac{\sqrt{l(l+1)-6}}{2}\delta(M_j = 3)\\
\langle l, 3|L_\mp|l, M_j\rangle &= -\,i\frac{\sqrt{l(l+1)-12}}{2}\delta(M_j = \bar{4}) - i\frac{\sqrt{l(l+1)-6}}{2}\delta(M_j = \bar{2})\\
&\quad \mp \frac{\sqrt{l(l+1)-6}}{2}\delta(M_j = 2) \pm \frac{\sqrt{l(l+1)-12}}{2}\delta(M_j = 4)\\
\langle l, \bar{3}|L_\mp|l, M_j\rangle &= \pm\frac{\sqrt{l(l+1)-12}}{2}\delta(M_j = \bar{4}) \mp \frac{\sqrt{l(l+1)-6}}{2}\delta(M_j = \bar{2})
\end{aligned}
$$

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$$+ i\frac{\sqrt{l(l+1)-6}}{2}\delta(M_j = 2) + i\frac{\sqrt{l(l+1)-12}}{2}\delta(M_j = 4).$$

Since the correct formulae were employed in the program, all the results are correct. This mistake was pointed out by Hyungjun Lee from Yonsei University (Korea).

(2) On page 8000, at the end of the first paragraph it states

> 'A hybrid option is to use frozen core methods, such as PAW[10] and FPLO[11], which will not be discussed here.'

where it should say

> 'A hybrid option is to use methods such as PAW[10] and FPLO [11], which will not be discussed here.'.