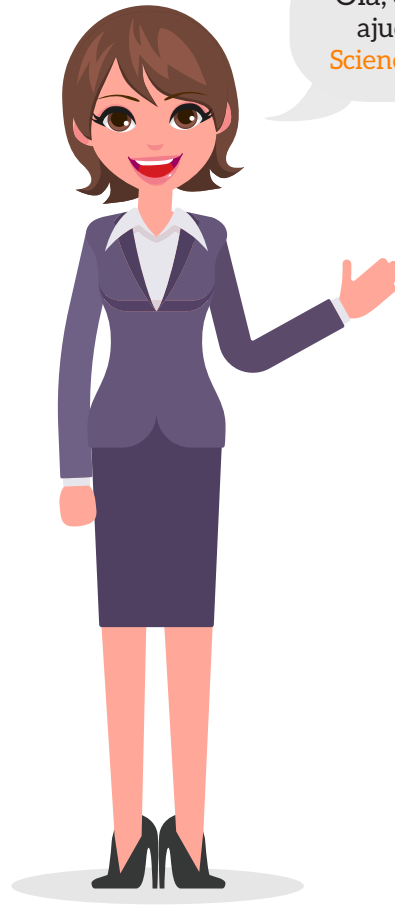




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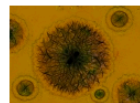
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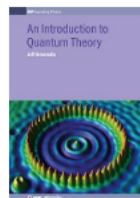
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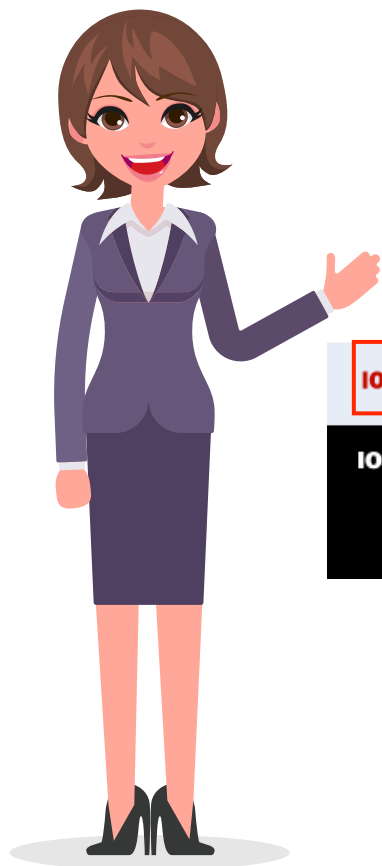
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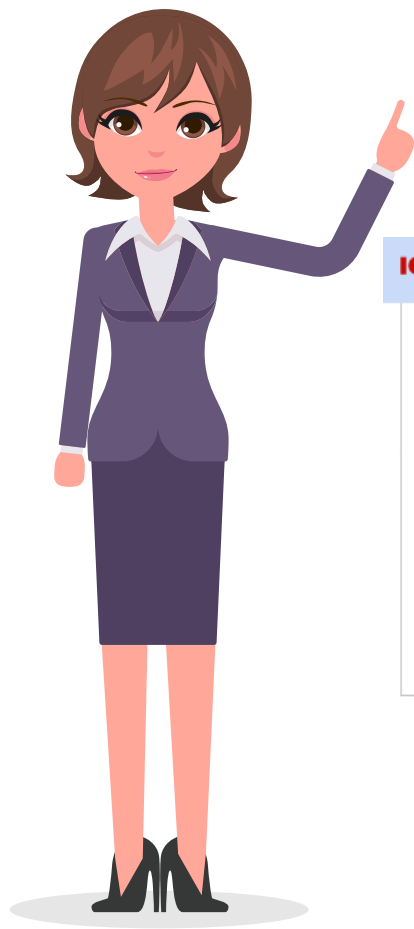
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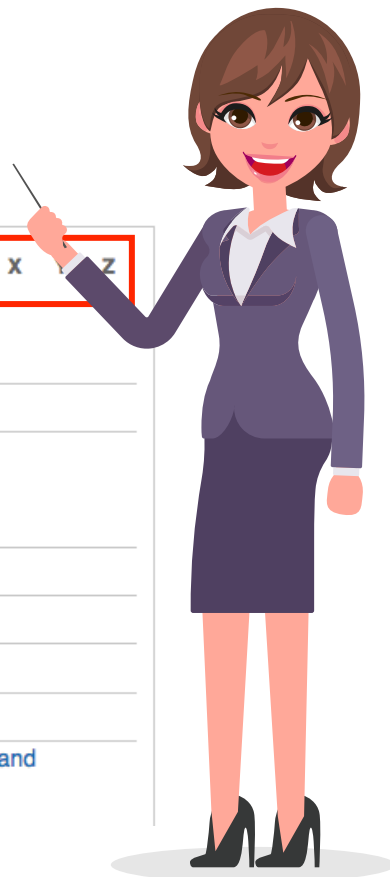
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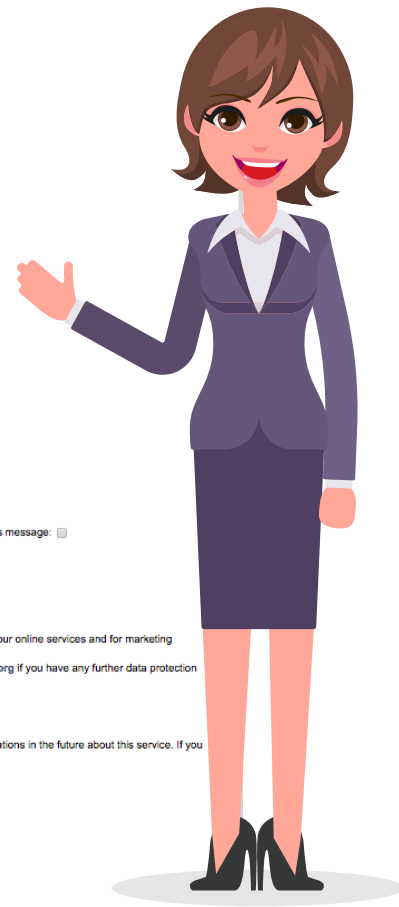
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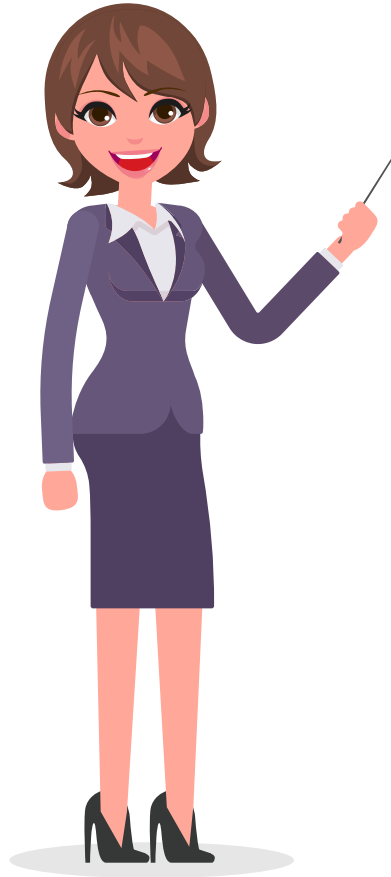
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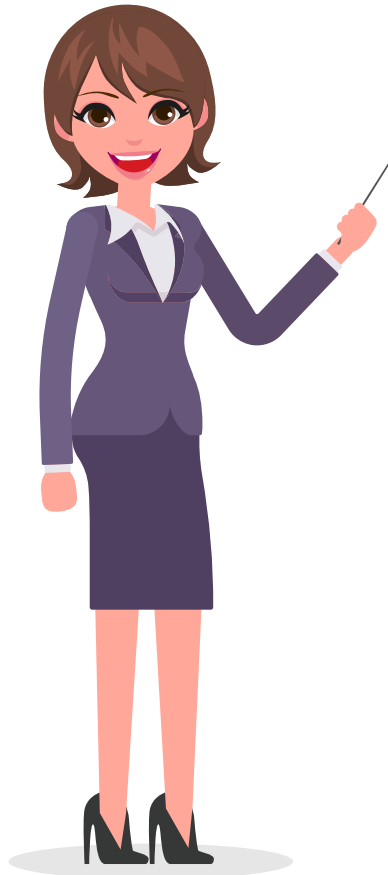
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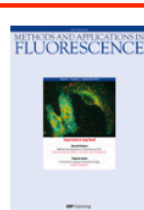
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John Cook<sup>1,2,3</sup>, Dana Nuccitelli<sup>2,4</sup>, Sarah A Green<sup>5</sup>, Mark Richardson<sup>6</sup>, Bärbel Winkler<sup>2</sup>, Rob Painting<sup>2</sup>, Robert Way<sup>7</sup>, Peter Jacobs<sup>8</sup> and Andrew Skuce<sup>2,9</sup>

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## Author e-mails

[j.cook3@uq.edu.au](mailto:j.cook3@uq.edu.au)

## Author affiliations

<sup>1</sup> Global Change Institute, University of Queensland, Australia

<sup>2</sup> Skeptical Science, Brisbane, Queensland, Australia

<sup>3</sup> School of Psychology, University of Western Australia, Australia

<sup>4</sup> Tetra Tech, Incorporated, McClellan, CA, USA

<sup>5</sup> Department of Chemistry, Michigan Technological University, USA

<sup>6</sup> Department of Meteorology, University of Reading, UK

<sup>7</sup> Department of Geography, Memorial University of Newfoundland, Canada

<sup>8</sup> Department of Environmental Science and Policy, George Mason University, USA

<sup>9</sup> Salt Spring Consulting Ltd, Salt Spring Island, BC, Canada

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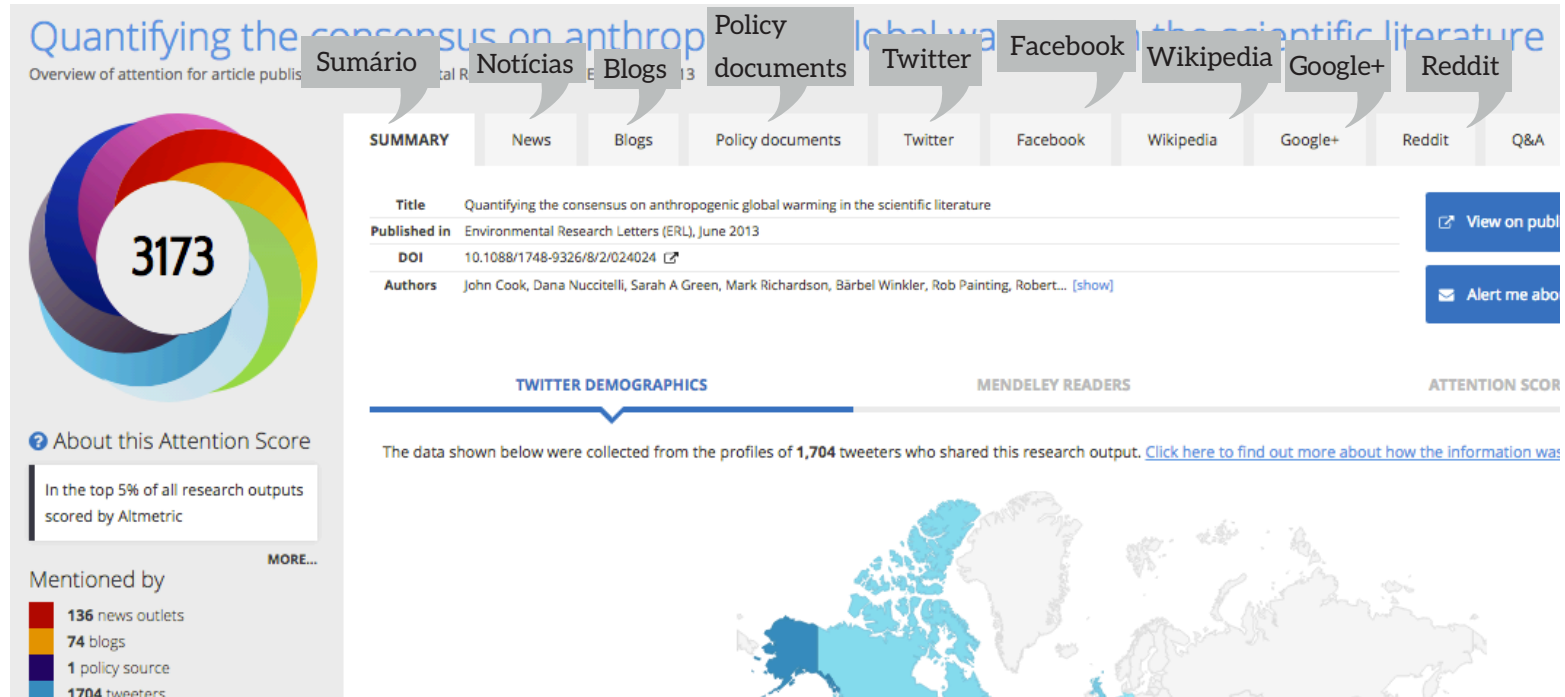
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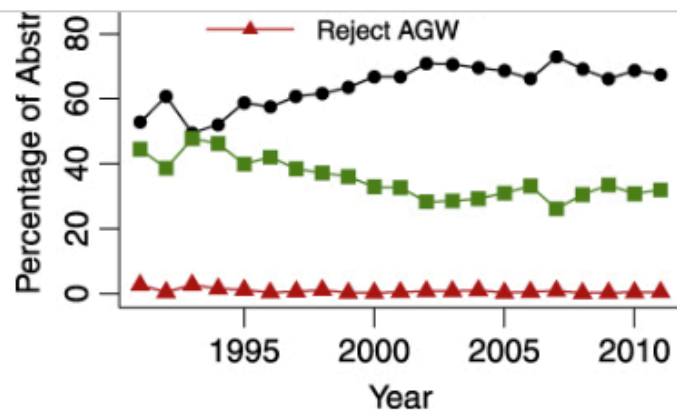





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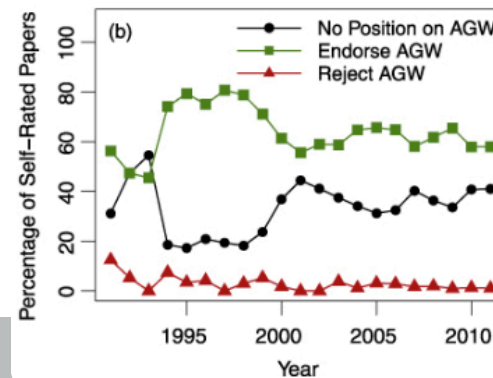
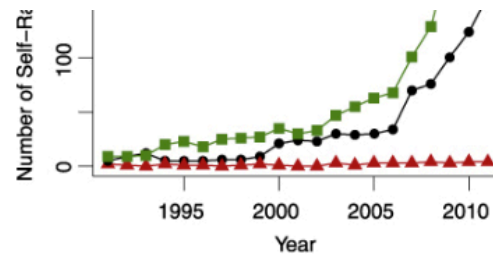
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sublattice model (Fähnle *et al* 1993). Within this model, one divides the crystal lattice into two sublattices, one composed of RE elements and the other of TM elements only (see figure 2). If the crystal structure of interest has only one crystallographic site for RE atoms, there are two spin states with energies  $E_1$  and  $E_2$  (see figure 3) which need to be computed for every stoichiometry to get an estimate for the  $J_{\text{RT}}$  integrals according to

$$J_{\text{RT}} = \frac{E_1 - E_2}{4S_{\text{R}}\bar{S}_{\text{T}}Z_{\text{RT}}Z_{\text{R}}}, \quad (1)$$

where  $E_1$  and  $E_2$  are the total energies of the parallel and antiparallel spin states (see figure 3),  $S_{\text{R}}$  is the magnetic spin moment of the RE sublattice,  $\bar{S}_{\text{T}}$  is the averaged magnetic spin moment of the TM

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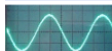
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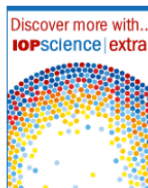
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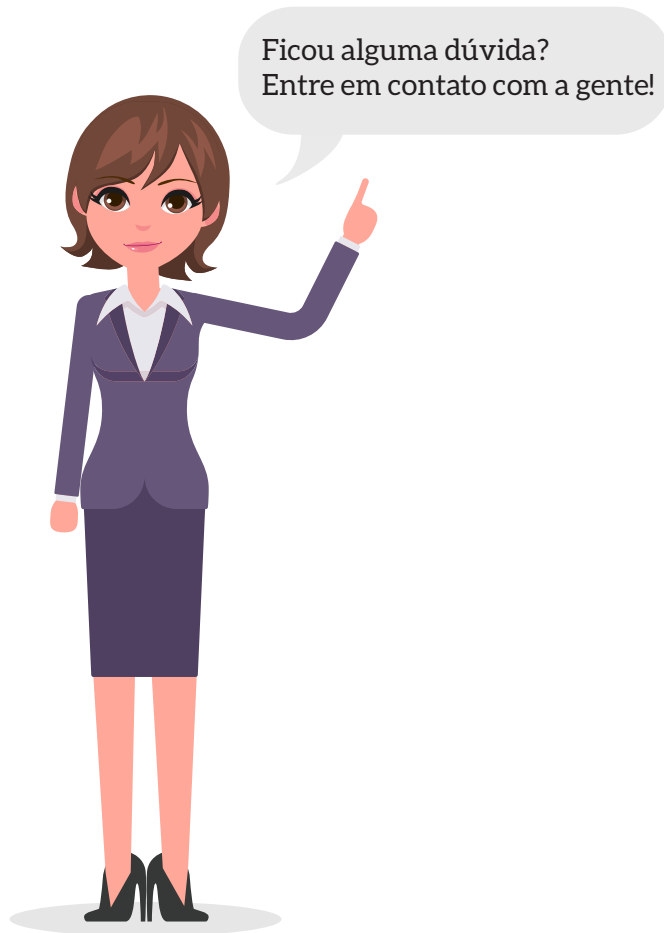
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