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Prof. Vegge has authored >125 peer-reviewed articles that are cited more than 5800 times and has an H-index of 39 (Google Scholar) in the area of atomic-scale computational techniques, which enable accelerated computational materials design, while maintaining predictive accuracy and providing calculational error-bars on the predictions. These techniques are typically developed and applied in close collaboration with leading experimental group and/or industry in a range of national and international projects, e.g., within the development of next-generation battery materials and concepts, and the design of efficient electrocatalysts for sustainable production of synthetic fuels and chemicals.