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Hydrogen and oxygen trapping at the H-cluster of [FeFe]'hydrogenase revealed by site-selective spectroscopy and QM/MM calculations

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## **ACCEPTED MANUSCRIPT**

### Hydrogen and oxygen trapping at the H-cluster of [FeFe]-hydrogenase revealed by siteselective spectroscopy and QM/MM calculations

Stefan Mebs<sup>1</sup>, Ramona Kositzki<sup>1</sup>, Jifu Duan<sup>2</sup>, Moritz Senger<sup>3</sup>, Florian Wittkamp<sup>4</sup>, Ulf-Peter Apfel<sup>4</sup>, Thomas Happe<sup>2</sup>, Sven T. Stripp<sup>3</sup>, Martin Winkler<sup>2\*</sup>, and Michael Haumann<sup>1\*</sup>

<sup>1</sup>Department of Physics, Biophysics of Metalloenzymes, Freie Universität Berlin, 14195 Berlin, Germany

Bernin, Germany

<sup>2</sup>Department of Biochemistry of Plants, Photobiotechnology, Ruhr-Universität Bochum,

44801 Bochum, Germany

<sup>3</sup>Department of Physics, Experimental Molecular Biophysics, Freie Universität Berlin, 14195 Berlin, Germany

<sup>4</sup>Department of Chemistry and Biochemistry, Inorganic Chemistry I, Ruhr-Universität

Bochum, 44801 Bochum, Germany

#### \*Correspondence to:

Dr. Michael Haumann, Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany, Phone: +49 30 838 56101, Email: michael.haumann@fu-berlin.de Dr. Martin Winkler, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany, +49 234 3227 049, Email: martin.winkler-2@rub.de

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**Keywords:** [FeFe]-hydrogenase, H-cluster, ligand binding, site-selective spectroscopy, QM/MM

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