

Publications of Stewart F. Parker

- (448) “In-situ real-time neutron imaging of gaseous H₂ adsorption and D₂ exchange on carbon-supported Pd catalysts”, H. Cavaye, C. Ballas, W. Kockelmann, D. Lennon, P. Collier, A.P.E. York, P.W. Albers, S.F. Parker, *Chemical Communications*, submitted for publication.
- (447) “The adsorption of nitrobenzene over an alumina-supported palladium catalyst: an infrared spectroscopic study”, A.M. McCullagh, E.K. Gibson, S.F. Parker, K. Refson and D. Lennon, *Physical Chemistry Chemical Physics*, submitted for publication.
- (446) “On the transition to gasoline-to-olefins chemistry in the cracking reactions of 1-octene over H-ZSM-5 catalysts”, A.P. Hawkins, A. Zachariou, S.F. Parker, P. Collier, N.S. Barrow, R.F. Howe and D. Lennon, *Applied Catalysis A: General*, submitted for publication.
- (445) “CO₂-mineralization and carbonation reactor rig: design and validation for in situ neutron scattering experiments - Engineering and lessons learned”, A. Mortazavi, M. Dudman, M. Evans, R. Copcutt, G. Romanelli, F. Demmel, D.H. Farrar, S.F. Parker, K.V. Tian, D. Di Tommaso, G.A. Chass, *Review of Scientific Instruments*, accepted for publication.
- (444) “Hydrogen spillover in tungsten oxide bronzes as observed by broadband neutron spectroscopy”, E. Lalik, S.F. Parker, G. Irvine, I. da Silva, M. Gutmann, G. Romanelli, K. Druzicki, R. Kosydar and M. Krzystyniak, *Energies* 16 (2023) 5496 [doi: 10.3390/en16145496] **Gold OA**
- (443) “Centrohexaindane, a unique polyaromatic hydrocarbon bearing the rare C^q(C^q)₄ core: Inelastic neutron scattering, infrared and Raman spectroscopy”, S.F. Parker, A.D. Fortes, D.W. Nye, S.J. Day and D. Kuck, *Chemistry – A European Journal* (2023) [doi: 10.1002/chem.202302057] **Gold OA**
- (442) “Neutron scattering studies of heterogeneous catalysis”, X. Yu, Y. Cheng, Y. Li, F. Polo-Garzon, J. Liu, E. Mamontov, M. Li, D. Lennon, S.F. Parker, A.J. Ramirez–Cuesta and Z. Wu, *Chemical Reviews* 123 (2023) 8638–8700 [doi: 10.1021/acs.chemrev.3c00101] **Gold OA**.
- (441) “A multi-wavelength Raman study of some oligothiophenes and polythiophene”, S.F. Parker, J.E. Trevelyan, T. Smith and K.P.J. Williams, *Physchem* 3 (2023) 210–219. [doi: 0.3390/physchem3020014] **Gold OA**
- (440) “Neutron scattering studies of the methanol-to-hydrocarbons reaction”, A. Zachariou, A.P. Hawkins, P. Collier, R.F. Howe, S.F. Parker and D. Lennon, *Catalysis Science & Technology* 13 (2023) 1976-1990 [doi: 10.1039/D2CY02154D]. **Gold OA**
- (439) “Vibrational spectra of neutral and doped oligothiophenes and polythiophene”, S.F. Parker, J.E. Trevelyan and H. Cavaye, *RSC Advances* 13 (2023) 5419-5427 [doi: 10.1039/D2RA07625J]. **Gold OA**
- (438) “In-situ anaerobic heating of human bones probed by neutron diffraction”, G. Festa, A.P. Mamede, D. Gonçalves, E. Cunha, W. Kockelmann, S.F. Parker, L.A.E. Batista de Carvalho and M.P.M. Marques, *Analytical Chemistry* 95 (2023) 2469–2477 [doi: 10.1021/acs.analchem.2c04721] **Gold OA**

- (437) “Computational and experimental studies of sulfided NiMo/Al-PILC: Catalyst activation and guaiacol adsorption sites on Mo- and Ni-edges”, F. Oemry, I. Adilina, W. Cahyanto, N. Rinaldi, F. Aulia, A. Jackson, S.F. Parker, A. Kroner and E. Shotton, *Physical Chemistry Chemical Physics* 25 (2023) 2978-2989 [doi: 10.1039/D2CP03987G].
- (436) “Overview of planned upgrade to the secondary spectrometer of TOSCA”, A. Perrichon, C. Bovo, S.F. Parker, D. Raspino, J. Armstrong and V. García Sakai, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 1047 (2023) 167899 [doi: 10.1016/j.nima.2022.167899] **Gold OA**
- (435) “Structural dynamics of chloromethanes through computational spectroscopy: combining INS and DFT”, M.M. Nolasco, M.M. Coimbra, S.F. Parker, P.D. Vaz and P.J.A. Ribeiro-Claro, *Molecules* 27 (2022) 7661 [doi: 10.3390/molecules27217661] **Gold OA**
- (434) “Counting the acid sites in a commercial ZSM-5 zeolite catalyst”, A. Zachariou, A.P. Hawkins, R.F. Howe, J. Skakle, P. Collier, N.S. Barrow, D. Nye, R. Smith, G. Stenning, S.F. Parker and D. Lennon, *ACS Physical Chemistry Au* 3 (2023) 74-83 [doi: 10.1021/acspchemau.2c00040] **Gold OA**
- (433) “Combining quasielastic neutron scattering and molecular dynamics to study methane motions in ZSM-5”, A.P. Hawkins, A. Zachariou, I.P. Silverwood, C. Yong, P. Collier, I. Todorov, R.F. Howe, S.F. Parker and D. Lennon, *Journal of Chemical Physics* 157 (2022) 184702 [doi: 10.1063/5.0123434] **Gold OA**
- (432) “Neutron-enhanced information on the laboratory characterization of ancient Egyptian leathers: hydration and preservation status”, G. Romanelli, C. Andreani, E. Ferraris, C. Greco, S. Ikram, S. Licoccia, G. Paladini, S.F. Parker, E. Preziosi, R. Senesi, L. Skinner, A.J. Veldmeijer, V. Venuti and V. Turina, *Information* 13 (2022) 467 [doi: 10.3390/info13100467] **Gold OA**
- (431) “Structure and spectroscopy of iron pentacarbonyl, Fe(CO)₅”, A.D. Fortes and S.F. Parker, *Journal of the American Chemical Society* 144 (2022) 17376–17386 [doi: 10.1021/jacs.2c01469] **Gold OA**
- (430) “The spontaneous self-assembly of a molecular water pipe in 3-D space”, I.R. Butler, D.M. Evans, P.N. Horton, S.J. Coles, S.F. Parker and S.C. Capelli, *IUCrJ* 9 (2022) 364-369 [doi: 10.1107/S2052252522003396] **Gold OA**
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- (428) “Assignment of the vibrational spectra of diiron nonacarbonyl, Fe₂(CO)₉”, S.F. Parker, *Physchem* 2 (2022) 108–115 [doi: 10.3390/physchem2020008] **Gold OA**
- (427) “Vibrational spectroscopy to investigate the ancient-Roman heat-modified skeletal remains at the Hypogeum of Garlands”, G. Festa, M. Rubini, P. Zaio, A. Gozzi, N. Libianchi, S.F. Parker, G. Romanelli, L.A.E. Batista de Carvalho and M.P.M. Marques, *Scientific Reports* 12 (2022) 3707. [doi: 10.1038/s41598-022-07689-0] **Gold OA**

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- (423) “Water in deep eutectic solvents: new insights from inelastic neutron scattering spectroscopy”, M.M. Nolasco, S.N. Pedro, C. Vilela, P.M.D. Vaz, P. Ribeiro-Claro, S. Rudić, S.F. Parker, C.S. da Rocha Freire, M.G. Freire and A.J.D. Silvestre, *Frontiers in Physics*. 10 (2022) 834571. [doi: 10.3389/fphy.2022.834571] **Gold OA**
- (422) “Understanding the surface characteristics of biochar and its catalytic activity for the hydrodeoxygenation of guaiacol”, I.B. Adilina, R.R. Widjaya, L. N. Hidayati, E. Supriadi, M. Safaat, F. Oemry, E. Restiawaty, Y. Bindar and S.F. Parker, *Catalysts* 11 (2021) 1434. [doi: 10.3390/catal11121434] **Gold OA**
- (421) “Exploiting the flexibility of the pyrochlore composition for acid-resilient iridium oxide electrocatalysts in proton exchange membranes”, D.L. Burnett, E. Petrucco, R.J. Kashtiban, S.F. Parker, J.D.B. Sharman and R.I. Walton, *Journal of Materials Chemistry A* 9 (2021) 25114–25127 [doi: 10.1039/D1TA05457K] **Gold OA**
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- (409) “New spectroscopic insight into the deactivation of a ZSM-5 methanol-to-hydrocarbons catalyst”, A. Zachariou, A.P. Hawkins, Suwardiyanto, P. Collier, N. Barrow, R.F. Howe, S.F. Parker and D. Lennon, *ChemCatChem* 13 (2021) 2625–2633 [doi: 10.1002/cctc.202100286] **Gold OA**
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