# Etienne Balan

List of Publications by Year
in descending order



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|---|---|---|---|
| 116 papers | 4,464 citations | 76326 40 h-index | 123424 61 g-index |
| 116 all docs | 116 docs citations | 116 times ranked | 4331 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | First-principles modeling of the infrared spectrum of kaolinite. American Mineralogist, 2001, 86, 1321-1330. | 1.9 | 201 |
| 2 | Incomplete retention of radiation damage in zircon from Sri Lanka. American Mineralogist, 2004, 89, 219-231. | 1.9 | 193 |
| 3 | Equilibrium isotopic fractionation in the kaolinite, quartz, water system: Prediction from first-principles density-functional theory. Geochimica Et Cosmochimica Acta, 2007, 71, 3170-3181. | 3.9 | 180 |
| 4 | Iron isotope fractionation between pyrite (FeS2), hematite (Fe2O3) and siderite (FeCO3): A first-principles density functional theory study. Geochimica Et Cosmochimica Acta, 2009, 73, 6565-6578. | 3.9 | 173 |
| 5 | Structural control over equilibrium silicon and oxygen isotopic fractionation: A first-principles density-functional theory study. Chemical Geology, 2009, 258, 28-37. | 3.3 | 128 |
| 6 | Metamictization and chemical durability of detrital zircon. American Mineralogist, 2001, 86, 1025-1033. | 1.9 | 124 |
| 7 | First-principles study of the OH-stretching modes of gibbsite. American Mineralogist, 2006, 91, 115-119. | 1.9 | 115 |
| 8 | 57 Fe MÃ¶ssbauer spectroscopy of tektites. Physics and Chemistry of Minerals, 1999, 26, 530-538. | 0.8 | 99 |
| 9 | First-principles study of OH-stretching modes in kaolinite, dickite, and nacrite. American Mineralogist, 2005, 90, 50-60. | 1.9 | 83 |
| 10 | Structural Fe3+ in Natural Kaolinites: New Insights from Electron Paramagnetic Resonance Spectra Fitting at X and Q-Band Frequencies. Clays and Clay Minerals, 1999, 47, 605-616. | 1.3 | 78 |
| 11 | Equilibrium Fractionation of Non-traditional Isotopes: a Molecular Modeling Perspective. Reviews in Mineralogy and Geochemistry, 2017, 82, 27-63. | 4.8 | 71 |
| 12 | Theoretical infrared spectrum of OH-defects in forsterite. European Journal of Mineralogy, 2011, 23, 285-292. | 1.3 | 69 |
| 13 | A carbonate-fluoride defect model for carbonate-rich fluorapatite. American Mineralogist, 2013, 98, 1066-1069. | 1.9 | 69 |
| 14 | Line-broadening effects in the powder infrared spectrum of apatite. Physics and Chemistry of Minerals, 2011, 38, 111-122. | 0.8 | 68 |
| 15 | Equilibrium zinc isotope fractionation in Zn-bearing minerals from first-principlesÂcalculations. Chemical Geology, 2016, 443, 87-96. | 3.3 | 68 |
| 16 | First-principles calculation of the infrared spectrum of lizardite. American Mineralogist, 2002, 87, 1286-1290. | 1.9 | 66 |
| 17 | V oxidation state in Feâ€“Ti oxides by high-energy resolution fluorescence-detected X-ray absorption spectroscopy. Physics and Chemistry of Minerals, 2011, 38, 449-458. | 0.8 | 65 |
| 18 | Anharmonicity of inner-OH stretching modes in hydrous phyllosilicates: assessment from first-principles frozen-phonon calculations. Physics and Chemistry of Minerals, 2007, 34, 621-625. | 0.8 | 62 |

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|---|---|---|---|
| 19 | The effect of radiation damage on local structure in the crystalline fraction of ZrSiO<sub>4</sub>: Investigating the<sup>29</sup>Si NMR response to pressure in zircon and reidite. American Mineralogist, 2003, 88, 1663-1667. | 1.9 | 61 |
| 20 | The oxidation state of vanadium in titanomagnetite from layered basic intrusions. American Mineralogist, 2006, 91, 953-956. | 1.9 | 61 |
| 21 | First-principles calculation of the infrared spectrum of hematite. American Mineralogist, 2008, 93, 1019-1027. | 1.9 | 61 |
| 22 | Preservation assessment of Mioceneâ€“Pliocene tooth enamel from Tugen Hills (Kenyan Rift Valley) through FTIR, chemical and stable-isotope analyses. Journal of Archaeological Science, 2010, 37, 1690-1699. | 2.4 | 57 |
| 23 | Surface modes in the infrared spectrum of hydrous minerals: the OH stretching modes of bayerite. Physics and Chemistry of Minerals, 2008, 35, 279-285. | 0.8 | 55 |
| 24 | First-principles calculation of H/D isotopic fractionation between hydrous minerals and water. Geochimica Et Cosmochimica Acta, 2010, 74, 3874-3882. | 3.9 | 55 |
| 25 | Equilibrium magnesium isotope fractionation between aqueous Mg2+ and carbonate minerals: Insights from path integral molecular dynamics. Geochimica Et Cosmochimica Acta, 2015, 163, 126-139. | 3.9 | 55 |
| 26 | Formation and evolution of lateritic profiles in the middle Amazon basin: Insights from radiation-induced defects in kaolinite. Geochimica Et Cosmochimica Acta, 2005, 69, 2193-2204. | 3.9 | 54 |
| 27 | Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 2008, 93, 950-953. | 1.9 | 54 |
| 28 | Transformation of haematite and Al-poor goethite to Al-rich goethite and associated yellowing in a ferralitic clay soil profile of the middle Amazon Basin (Manaus, Brazil). European Journal of Soil Science, 2005, 56, 575-588. | 3.9 | 53 |
| 29 | First-principles study of boron speciation in calcite and aragonite. Geochimica Et Cosmochimica Acta, 2016, 193, 119-131. | 3.9 | 52 |
| 30 | New Insights in the Ontogeny and Taphonomy of the Devonian Acanthodian Triazeugacanthus affinis From the Miguasha Fossil-LagerstÃtte, Eastern Canada. Minerals (Basel, Switzerland), 2016, 6, 1. | 2.0 | 51 |
| 31 | X-ray linear dichroism in cubic compounds: The case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mtext>Cr</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msup></mml:mrow></mml:math>:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgAl</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>4</mml:mtext></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>, Physical Review B, 2008, 78, . | 3.2 | 50 |
| 32 | Evolution of the macromolecular structure of sporopollenin during thermal degradation. Heliyon, 2015, 1, e00034. | 3.2 | 48 |
| 33 | Surface chemistry of weathered zircons. Chemical Geology, 2001, 181, 13-22. | 3.3 | 47 |
| 34 | Reaction mechanisms in swelling clays under ionizing radiation: influence of the water amount and of the nature of the clay mineral. RSC Advances, 2017, 7, 526-534. | 3.6 | 47 |
| 35 | Low-temperature infrared spectroscopic study of OH-stretching modes in kaolinite and dickite. American Mineralogist, 2010, 95, 1257-1266. | 1.9 | 45 |
| 36 | Incorporation of water in iron-free ringwoodite: A first-principles study. American Mineralogist, 2009, 94, 83-89. | 1.9 | 44 |

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|---|---|---|---|
| 37 | Dissolution of radiation-damaged zircon in lateritic soils. American Mineralogist, 2007, 92, 1978-1989. | 1.9 | 43 |
| 38 | Elasticity of serpentines and extensive serpentinization in subduction zones. Geophysical Research Letters, 2007, 34, . | 4.0 | 42 |
| 39 | Clumped fluoride-hydroxyl defects in forsterite: Implications for the upper-mantle. Earth and Planetary Science Letters, 2014, 390, 287-295. | 4.4 | 42 |
| 40 | First-principles simulation of arsenate adsorption on the (1<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 637 Td (xmlns:mml="http:/ surface of hematite. Geochimica Et Cosmochimica Acta, 2012, 86, 182-195. | 3.9 | 40 |
| 41 | Quantitative Measurement of Paramagnetic Fe3+ in Kaolinite. Clays and Clay Minerals, 2000, 48, 439-445. | 1.3 | 39 |
| 42 | First-principles investigation of equilibrium isotopic fractionation of O- and Si-isotopes between refractory solids and gases in the solar nebula. Earth and Planetary Science Letters, 2012, 319-320, 118-127. | 4.4 | 39 |
| 43 | Strong electric fields at a prototypical oxide/water interface probed by ab initio molecular dynamics: MgO(001). Physical Chemistry Chemical Physics, 2015, 17, 20382-20390. | 2.8 | 39 |
| 44 | Effect of iron and trivalent cations on OH defects in olivine. American Mineralogist, 2017, 102, 302-311. | 1.9 | 39 |
| 45 | Reduced partition function ratios of iron and oxygen in goethite. Geochimica Et Cosmochimica Acta, 2015, 151, 19-33. | 3.9 | 38 |
| 46 | Behavior of Paramagnetic Iron during the Thermal Transformations of Kaolinite. Journal of the American Ceramic Society, 2001, 84, 1017-1024. | 3.8 | 36 |
| 47 | Lateritic and redoximorphic features in a faulted landscape near Manaus, Brazil. European Journal of Soil Science, 2002, 53, 203-217. | 3.9 | 36 |
| 48 | Deciphering the weathering processes using environmental mineralogy and geochemistry: Towards an integrated model of laterite and podzol genesis in the Upper Amazon Basin. Comptes Rendus - Geoscience, 2011, 343, 188-198. | 1.2 | 35 |
| 49 | Hydrogen isotope determination by TC/EA technique in application to volcanic glass as a window into secondary hydration. Journal of Volcanology and Geothermal Research, 2017, 348, 49-61. | 2.1 | 35 |
| 50 | Combined dating of goethites and kaolinites from ferruginous duricrusts. Deciphering the Late Neogene erosion history of Central Amazonia. Chemical Geology, 2018, 479, 136-150. | 3.3 | 35 |
| 51 | Multiple Ionic-Plasmon Resonances in Naturally Occurring Multiwall Nanotubes: Infrared Spectra of Chrysotile Asbestos. Physical Review Letters, 2002, 89, 177401. | 7.8 | 34 |
| 52 | Theoretical isotopic fractionation between structural boron in carbonates and aqueous boric acid and borate ion. Geochimica Et Cosmochimica Acta, 2018, 222, 117-129. | 3.9 | 33 |
| 53 | First-principles study of the structural and isotopic properties of Al- and OH-bearing hematite. Geochimica Et Cosmochimica Acta, 2010, 74, 3948-3962. | 3.9 | 32 |
| 54 | Radiation-induced defects in clay minerals: A review. Nuclear Instruments & Methods in Physics Research B, 2012, 277, 112-120. | 1.4 | 32 |

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| 55 | Inheritance <I>vs.</I> neoformation of kaolinite during lateritic soil formation: a case study in the middle Amazon Basin. Clays and Clay Minerals, 2007, 55, 253-259. | 1.3 | 30 |
| 56 | Low-temperature evolution of OH bands in synthetic forsterite, implication for the nature of H defects at high pressure. Physics and Chemistry of Minerals, 2013, 40, 499-510. | 0.8 | 30 |
| 57 | The aperiodic states of zircon: an ab initio molecular dynamics study. American Mineralogist, 2003, 88, 1769-1777. | 1.9 | 28 |
| 58 | Identification of hydrogen defects linked to boron substitution in synthetic forsterite and natural olivine. American Mineralogist, 2014, 99, 2138-2141. | 1.9 | 28 |
| 59 | First-principles modeling of sulfate incorporation and 34S/32S isotopic fractionation in different calcium carbonates. Chemical Geology, 2014, 374-375, 84-91. | 3.3 | 26 |
| 60 | Kaolin-Group Minerals: From Hydrogen-Bonded Layers to Environmental Recorders. Elements, 2014, 10, 183-188. | 0.5 | 26 |
| 61 | Equilibrium isotopic fractionation between aqueous Zn and minerals from first-principles calculations. Chemical Geology, 2018, 483, 342-350. | 3.3 | 26 |
| 62 | Induced modifications of kaolinite under ionizing radiation: an infrared spectroscopic study. Physics and Chemistry of Minerals, 2009, 36, 291-299. | 0.8 | 25 |
| 63 | Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics. Geochimica Et Cosmochimica Acta, 2014, 135, 203-216. | 3.9 | 25 |
| 64 | Modeling the attenuated total reflectance infrared (ATR-FTIR) spectrum of apatite. Physics and Chemistry of Minerals, 2016, 43, 615-626. | 0.8 | 25 |
| 65 | Reaction Mechanisms in Talc under Ionizing Radiation: Evidence of a High Stability of Hâ€¢ Atoms. Journal of Physical Chemistry C, 2016, 120, 2087-2095. | 3.1 | 25 |
| 66 | Probing atomic scale transformation of fossil dental enamel using Fourier transform infrared and nuclear magnetic resonance spectroscopy: A case study from the Tugen Hills (Rift Gregory, Kenya). Acta Biomaterialia, 2014, 10, 3952-3958. | 8.3 | 24 |
| 67 | Infrared spectroscopic properties of goethite: anharmonic broadening, long-range electrostatic effects and Al substitution. Physics and Chemistry of Minerals, 2014, 41, 289-302. | 0.8 | 24 |
| 68 | Radiation-induced defects in dickites from the El Berrocal granitic system (Spain): relation with past occurrence of natural radioelements. European Journal of Mineralogy, 2003, 15, 629-640. | 1.3 | 23 |
| 69 | Incorporation of Cr 3+ in dickite: a spectroscopic study. Physics and Chemistry of Minerals, 2002, 29, 273-279. | 0.8 | 22 |
| 70 | Experimental and theoretical study of the vibrational properties of diaspore (Î±-AlOOH). Physics and Chemistry of Minerals, 2012, 39, 93-102. | 0.8 | 22 |
| 71 | Comment on â€œNew data on equilibrium iron isotope fractionation among sulfides: Constraints on mechanisms of sulfide formation in hydrothermal and igneous systemsâ€•by V.B. Polyakov and D.M. Soultanov. Geochimica Et Cosmochimica Acta, 2012, 87, 356-359. | 3.9 | 21 |
| 72 | First-principles modeling of chlorine isotope fractionation between chloride-bearing molecules and minerals. Chemical Geology, 2019, 525, 424-434. | 3.3 | 21 |

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| 73 | Theoretical investigation of the anomalous equilibrium fractionation of multiple sulfur isotopes during adsorption. Earth and Planetary Science Letters, 2009, 284, 88-93. | 4.4 | 20 |
| 74 | Electronic structure and local environment of substitutional V3+ in grossular garnet Ca3Al2(SiO4)3: K-edge X-ray absorption spectroscopy and first-principles modeling. American Mineralogist, 2010, 95, 1161-1171. | 1.9 | 20 |
| 75 | Contribution of interstitial OH groups to the incorporation of water in forsterite. Physics and Chemistry of Minerals, 2014, 41, 105-114. | 0.8 | 20 |
| 76 | First-Principles Vibrational Electron Energy Loss Spectroscopy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math> -Guanine. Physical Review Letters, 2017, 119, 027402. | 7.8 | 19 |
| 77 | Boron isotopic fractionation during adsorption by calcite â€“ Implication for the seawater pH proxy. Geochimica Et Cosmochimica Acta, 2018, 240, 255-273. | 3.9 | 19 |
| 78 | Structure and theoretical infrared spectra of OH defects in quartz. European Journal of Mineralogy, 2020, 32, 311-323. | 1.3 | 19 |
| 79 | Theoretical study of OH-defects in pure enstatite. Physics and Chemistry of Minerals, 2013, 40, 41-50. | 0.8 | 18 |
| 80 | Unraveling weathering episodes in Tertiary regoliths by kaolinite dating (Western Ghats, India). Gondwana Research, 2019, 69, 89-105. | 6.0 | 18 |
| 81 | Insights into the high-pressure behavior of kaolinite from infrared spectroscopy and quantum-mechanical calculations. Physics and Chemistry of Minerals, 2012, 39, 143-151. | 0.8 | 16 |
| 82 | Iron bands, fragipans and duripans in the northeastern plateaus of Brazil â€” properties and genesis. Canadian Journal of Soil Science, 1998, 78, 519-530. | 1.2 | 15 |
| 83 | Theoretical Raman spectrum and anharmonicity of tetrahedral OH defects in hydrous forsterite. European Journal of Mineralogy, 2017, 29, 201-212. | 1.3 | 15 |
| 84 | New constraints on Xe incorporation mechanisms in olivine from first-principles calculations. Geochimica Et Cosmochimica Acta, 2018, 222, 146-155. | 3.9 | 14 |
| 85 | Radiation damage induced by krypton ions in sintered Î±-Al2O3. Radiation Protection Dosimetry, 2006, 119, 222-225. | 0.8 | 13 |
| 86 | Infrared signatures of OH-defects in wadsleyite: A first-principles study. American Mineralogist, 2013, 98, 2132-2143. | 1.9 | 13 |
| 87 | Theoretical infrared spectrum of partially protonated cationic vacancies in forsterite. European Journal of Mineralogy, 2014, 26, 203-210. | 1.3 | 13 |
| 88 | Infrared spectroscopic study of sulfate-bearing calcite from deep-sea bamboo coral. European Journal of Mineralogy, 2017, 29, 397-408. | 1.3 | 13 |
| 89 | Site-specific equilibrium isotopic fractionation of oxygen, carbon and calcium in apatite. Geochimica Et Cosmochimica Acta, 2017, 219, 57-73. | 3.9 | 13 |
| 90 | Spectroscopic investigation and theoretical modeling of kaolinite-group minerals and other low-temperature phases. Comptes Rendus - Geoscience, 2011, 343, 177-187. | 1.2 | 12 |

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| 91 | First-principles study of OH defects in zircon. Physics and Chemistry of Minerals, 2013, 40, 547-554. | 0.8 | 12 |
| 92 | Macroscopic electrostatic effects in ATR-FTIR spectra of modern and archeological bones. American Mineralogist, 2018, 103, 326-329. | 1.9 | 12 |
| 93 | Atomic scale transformation of bone in controlled aqueous alteration experiments. Palaeogeography, Palaeoclimatology, Palaeoecology, 2019, 526, 80-95. | 2.3 | 12 |
| 94 | Theoretical study of the local charge compensation and spectroscopic properties of B-type carbonate defects in apatite. Physics and Chemistry of Minerals, 2014, 41, 347-359. | 0.8 | 11 |
| 95 | Assessing bone transformation in late Miocene and Plioâ€Pleistocene deposits of Kenya and South Africa. Archaeometry, 2019, 61, 1129-1143. | 1.3 | 11 |
| 96 | Structural, textural, and chemical controls on the OH stretching vibrations in serpentine-group minerals. European Journal of Mineralogy, 2021, 33, 447-462. | 1.3 | 11 |
| 97 | Theoretical infrared spectra of OH defects in corundum (<i>Î±</i>-Al<sub>2</sub>O<sub>3</sub>). European Journal of Mineralogy, 2020, 32, 457-467. | 1.3 | 11 |
| 98 | First principles study of water adsorption on the (100) surface of zircon: Implications for zircon dissolution. American Mineralogist, 2001, 86, 910-914. | 1.9 | 10 |
| 99 | van der Waals Contribution to the Relative Stability of Aqueous Zn(2+) Coordination States. Journal of Chemical Theory and Computation, 2017, 13, 3340-3347. | 5.3 | 10 |
| 100 | Kaolinite dating from Acrisol and Ferralsol: A new key to understanding the landscape evolution in NW Amazonia (Brazil). Geoderma, 2020, 370, 114354. | 5.1 | 9 |
| 101 | Native Cd+ in sedimentary fluorapatite. European Journal of Mineralogy, 2002, 14, 1087-1094. | 1.3 | 8 |
| 102 | Influence of the nature of the gas phase on the degradation of RNA during fossilization processes. Applied Clay Science, 2020, 191, 105616. | 5.2 | 8 |
| 103 | Local mode interpretation of the OH overtone spectrum of 1:1 phyllosilicates. European Journal of Mineralogy, 2021, 33, 209-220. | 1.3 | 8 |
| 104 | Impact of UV Radiation on the Raman Signal of Cystine: Implications for the Detection of S-rich Organics on Mars. Astrobiology, 2021, 21, 566-574. | 3.0 | 8 |
| 105 | Tropical Weathering History Recorded in the Silicon Isotopes of Lateritic Weathering Profiles. Geophysical Research Letters, 2021, 48, e2021GL092957. | 4.0 | 7 |
| 106 | Application of Vibrational Spectroscopy to the Characterization of Phyllosilicates and other Industrial Minerals. , 0, , 171-226. | | 7 |
| 107 | Structure, reactivity and spectroscopic properties of minerals from lateritic soils: insights from ab initio calculations. European Journal of Soil Science, 2007, 58, 870-881. | 3.9 | 6 |
| 108 | First-principles modeling of the infrared spectrum of antigorite. European Journal of Mineralogy, 2021, 33, 389-400. | 1.3 | 6 |

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| 109 | Low-temperature infrared spectrum and atomic-scale structure of hydrous defects in diopside. European Journal of Mineralogy, 2020, 32, 505-520. | 1.3 | 6 |
| 110 | Dating kaolinite from the Neogene IÃ§Ã¡ Formation and overlying laterites, central Amazonia, Brazil: Constraints for a stratigraphic correlation. Palaeogeography, Palaeoclimatology, Palaeoecology, 2020, 554, 109818. | 2.3 | 5 |
| 111 | Line-broadening and anharmonic effects in the attenuated total reflectance infrared spectra of calcite. European Journal of Mineralogy, 2019, 31, 73-81. | 1.3 | 4 |
| 112 | First-principles modeling of the infrared spectrum of Fe- and Al-bearing lizardite. European Journal of Mineralogy, 2021, 33, 647-657. | 1.3 | 4 |
| 113 | Theoretical OH stretching vibrations in dravite. European Journal of Mineralogy, 2022, 34, 239-251. | 1.3 | 4 |
| 114 | Radiation-induced Defects in Nonradioactive Natural Minerals: Mineralogical and Environmental Significance. Materials Research Society Symposia Proceedings, 2003, 792, 22. | 0.1 | 1 |
| 115 | The determination of Ti<sub>2</sub>O<sub>3</sub>in titania slags: a comparison of different methods of analysis. Institutions of Mining and Metallurgy Transactions Section C: Mineral Processing and Extractive Metallurgy, 2008, 117, 166-170. | 0.6 | 1 |
| 116 | Vibrational spectroscopic study of three Mgâ€“Ni mineral series in white and greenish clay infillings of the New Caledonian Ni-silicate ores. European Journal of Mineralogy, 2021, 33, 743-763. | 1.3 | 0 |