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See Guillermo Restrepo, pp. 973–982. Image reproduced by permission of Thomas Endler from *Digital Discovery*, 2026, **5**, 973.

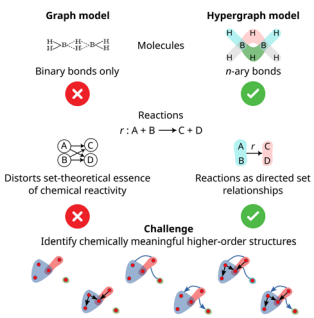
Inside cover
See Xingran Kou, Dachuan Zhang *et al.*, pp. 1068–1078. Image reproduced by permission of Xingran Kou from *Digital Discovery*, 2026, **5**, 1068. Image generated with Google Gemini Pro.

PERSPECTIVES

973

Higher order structures in chemistry: hypergraphs reshape the molecule and the reaction

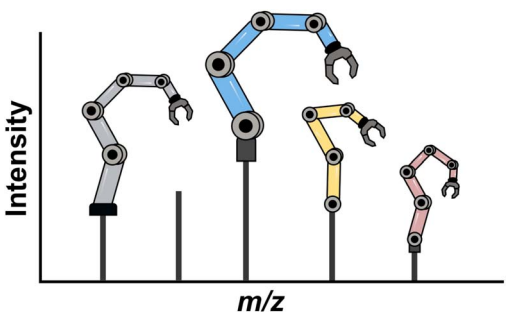
Guillermo Restrepo*



983

Automated and robotic sample delivery systems for mass spectrometry and ion-mobility spectrometry

Chikondi Shaba, Decibel P. Elpa and Pawel L. Urban*



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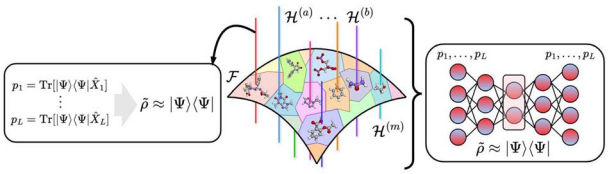
PERSPECTIVES

1011

Connecting the concepts of quantum state tomography and molecular representations for machine learning

Raul Ortega-Ochoa,* Luis Mantilla Calderón,* Juan Bernardo Perez Sanchez, Mohsen Bagherimehrab, Abdulrahman Aldossary, Tejs Vegge, Tonio Buonassisi and Alán Aspuru-Guzik*

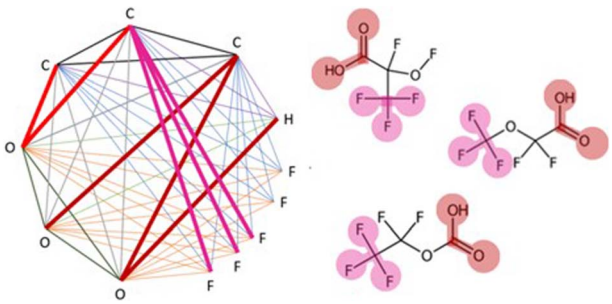


REVIEWS

1023

Advances and perspectives in computer-assisted structure elucidation: a review

Dagny Aurich and Emma L. Schymanski*



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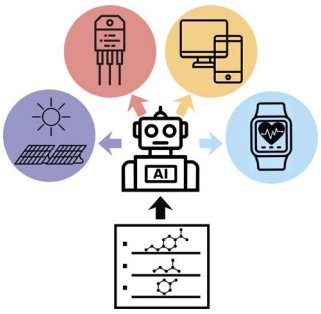
Artificial intelligence in the discovery and design of molecular semiconductors: a systematic review

Malin Zollner, Yashar Moshfeghi and Tahereh Nematiaram*



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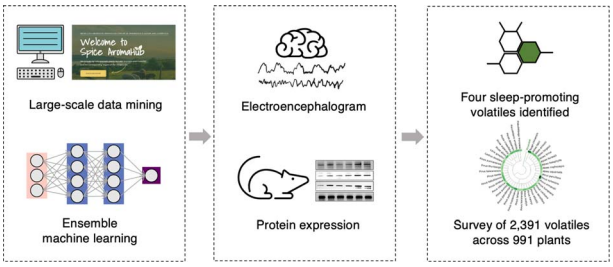
1068

Mapping sleep-promoting volatiles in aromatic plants with machine learning: a comprehensive survey of 2300 molecules

Peiqin Shi, Xing Huang, Qinfei Ke, Xingran Kou* and Dachuan Zhang*



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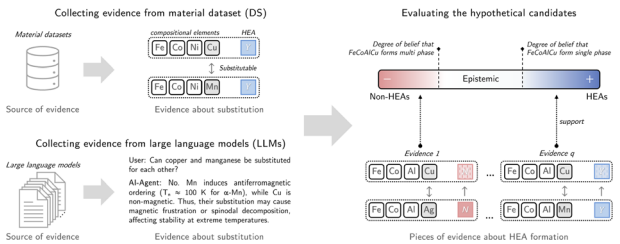
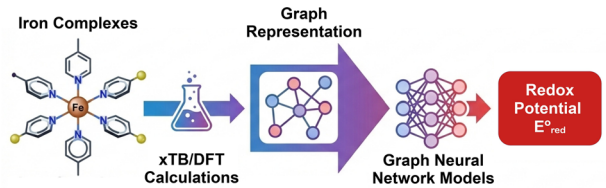


Beyond interpolation: integration of data and AI-extracted knowledge for high-entropy alloy discovery

Minh-Quyet Ha, Dinh-Khiet Le, Viet-Cuong Nguyen, Hiori Kino, Stefano Curtarolo and Hieu-Chi Dam*

1098



Redox potential prediction of Fe(II)/Fe(III) complexes: a density functional theory and graph neural network approach

Fakhrul H. Bhuiyan, Hassan Harb, Rajeev Surendran Assary and Álvaro Vázquez-Mayagoitia*

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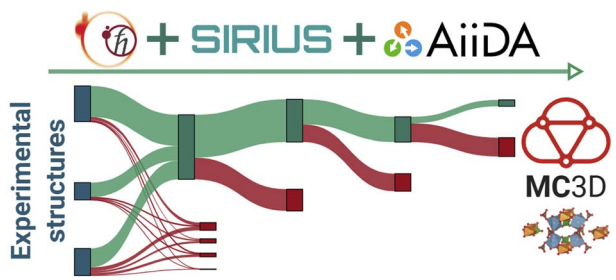
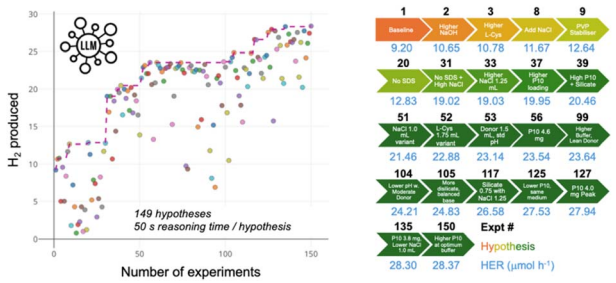


MC3D: the Materials Cloud computational database of experimentally known stoichiometric inorganics

Sebastiaan P. Huber, Michail Minotakis, Marnik Bercx, Timo Reents, Kristjan Eimre, Nataliya Paulish, Nicolas Hörmann, Martin Uhrin, Nicola Marzari and Giovanni Pizzi*

1132



Can we automate scientific reasoning in closed-loop experiments using large language models?

Abdoulatif Cissé, Max E. Cooper, Mengjia Zhu, Xenophon Evangelopoulos and Andrew I. Cooper*

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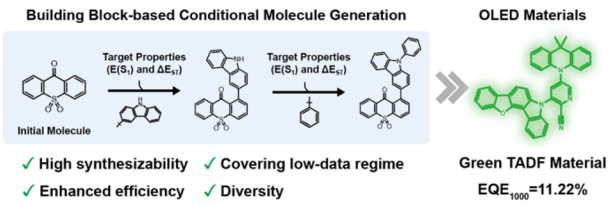
1161

Harnessing generative AI for efficient organic materials discovery in low-data regimes

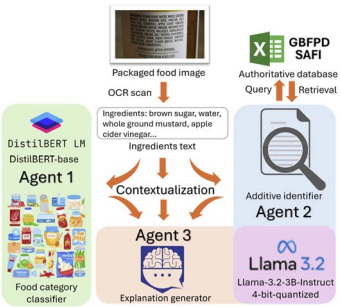
Jun Hyeong Kim, Kyunghoon Lee, Hyeonsu Kim, MinSoo Kang, Suk-Ku Chang, Yinglan Jin, Dongwook Kim and Woo Youn Kim*



1172

Food additive lens: an on-device AI application for real-time science-based consumer education on food additives using retrieval-augmented generation

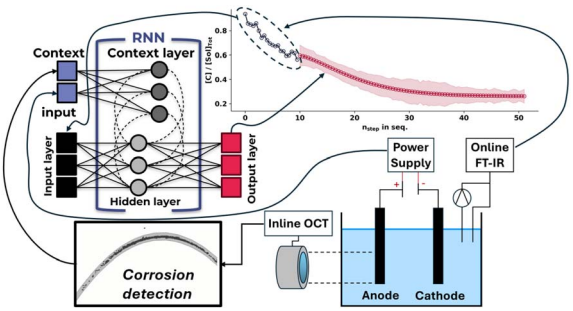
Yihang Feng, Yi Wang, Xinhao Wang, Bo Zhao, Jinbo Bi, Song Han* and Yangchao Luo*



1191

Machine learning-based time-series forecasting prevents electrode corrosion in organic electrochemistry

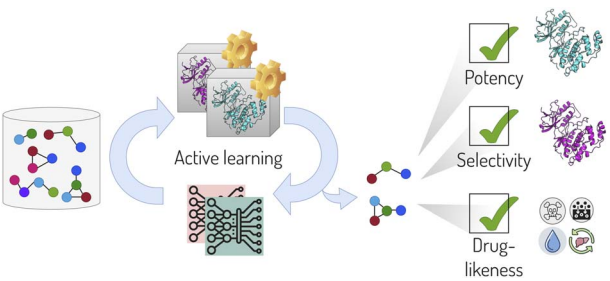
Josef Tausendschön,* Michael Poelzl, Nikola Petrovic, Jason D. Williams and Elisabeth Fink



1204

A simple compound prioritization method for drug discovery considering multi-target binding

Alžbeta Kubincová and David L. Mobley*



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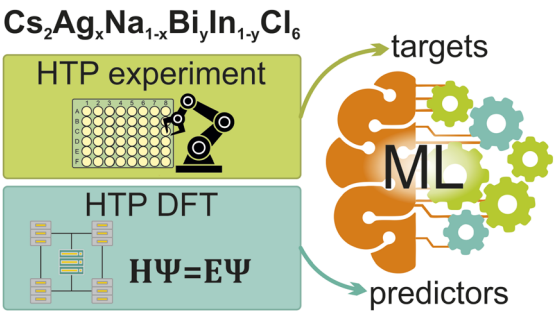

Towards an understanding of photoluminescence in lead-free $Cs_2Ag_xNa_{1-x}Bi_yIn_{1-y}Cl_6$ double perovskites by machine learning prediction from density functional theory ground state properties

Marina S. Günthert,* Larry Lüer, Oleksandr Stroyuk, Oleksandra Raievska, Christian Kupfer, Andres Osvet, Bernd Meyer and Christoph J. Brabec

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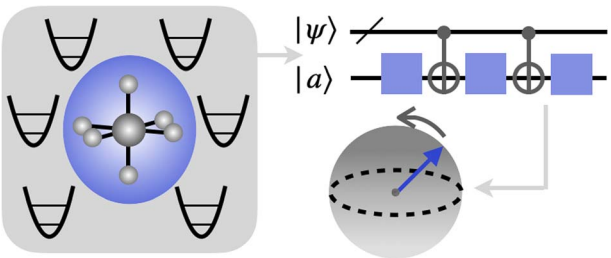
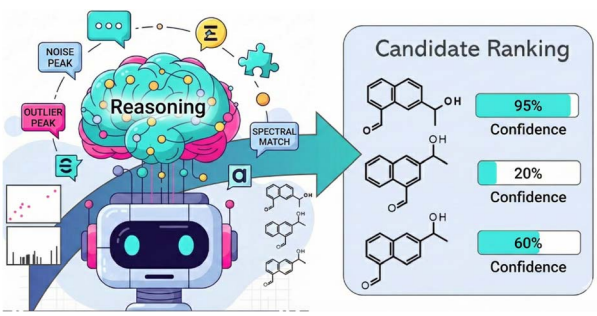


Mapping Bloch-Redfield dynamics into a unitary gate-based quantum algorithm

Koray Aydoğan, Maryam Abbasi, Whitney J. Short, Mikayla Z. Fahrenbruch, Timothy J. Krogmeier, Anthony W. Schlimgen and Kade Head-Marsden*

1237



Enhancing molecular structure elucidation with reasoning-capable LLMs

Martin Priessner,* Richard J. Lewis, Magnus J. Johansson, Jonathan M. Goodman, Jon Paul Janet and Anna Tomberg*

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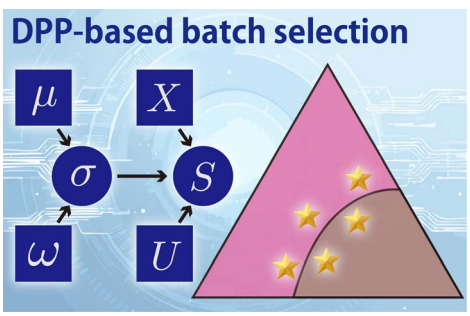

Bayesian diversity control for batch-based phase diagram determination

Peiheng Zou, Ryo Tamura and Koji Tsuda*

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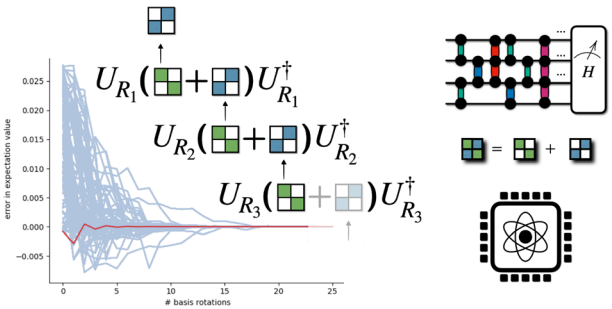
A physics-informed measurement protocol for expectation values of fermionic observables

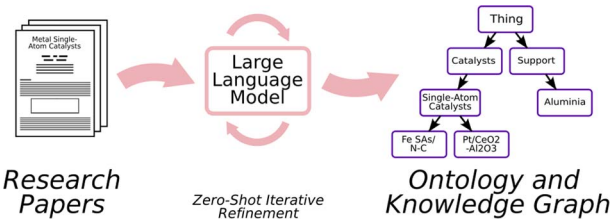
Davide Bincoletto and Jakob S. Kottmann*



1269

Scientific knowledge graph and ontology generation using open large language models

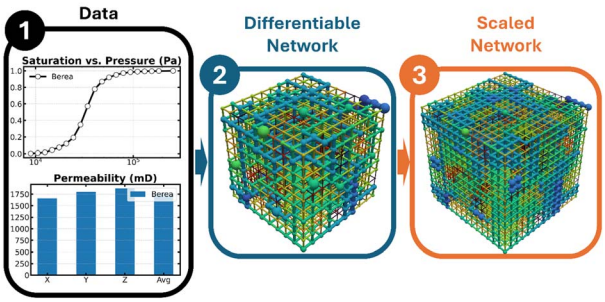
Alexandru Oarga, Matthew Hart, Andres M. Bran,* Magdalena Lederbauer and Philippe Schwaller*



1280

A fully differentiable pore network for digital reconstruction of porous media

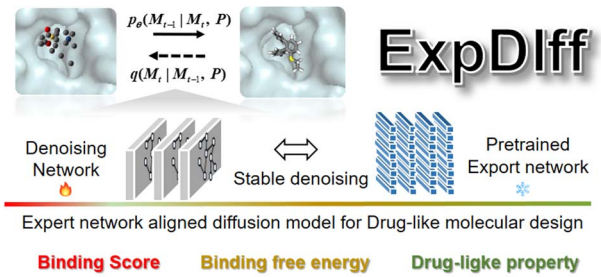
Michael McKague, Mohammad Mehrnia, Mohammad Amin Sadeghi and Jeff Gostick*



1296

A feature-aligned diffusion model for controllable generation of 3D drug-like molecules

Hao Lu, Zhiqiang Wei, Xiancong Hou, Wenzheng Han, Yang Zhang* and Hao Liu*



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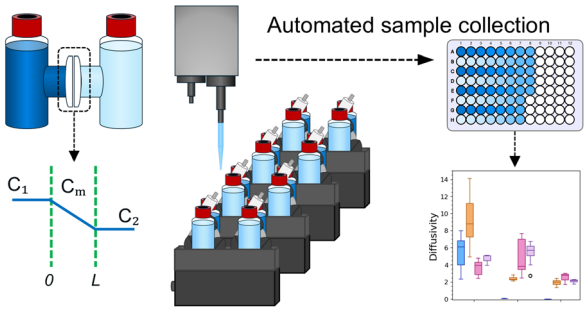

An automated sampling workflow for parallel long-term membrane diffusion cell testing

Claire Benstead, Maria Politi, David S. Bergsman* and Lilo D. Pozzo*

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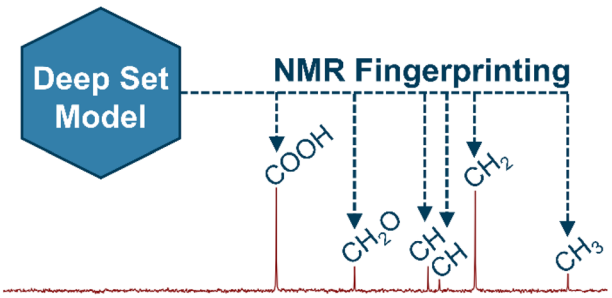

Deep set model for the automated NMR fingerprinting of unknown mixtures

Jens Wagner, Kerstin Münnemann, Thomas Specht, Hans Hasse and Fabian Jirasek*

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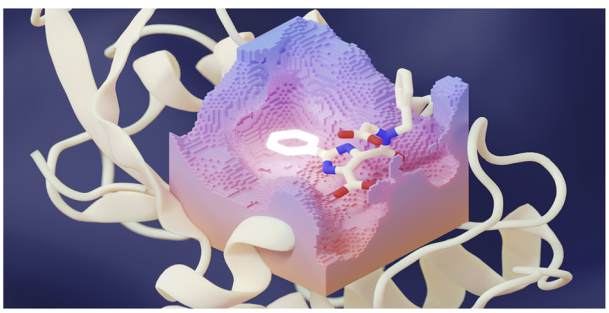

Precision fragment addition: domain-specific DeepFrag2 models for smarter lead optimization

César R. García-Jacas, Harrison Green, Shayne D. Wierbowski and Jacob D. Durrant*

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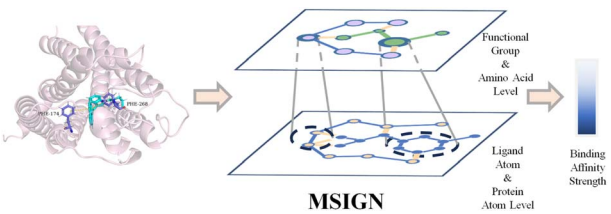

MSIGN: A deep learning framework based on multi-scale interaction graph neural networks for predicting binding of synthetic cannabinoids to receptors

Zhenyong Cheng, Dinghao Liu, Yuanpeng Fu, Kewei Sheng, Yan Xing, Yanling Qiao, Shangxuan Cai, Jubo Wang, Peng Xu, Bin Di and Jun Liao*

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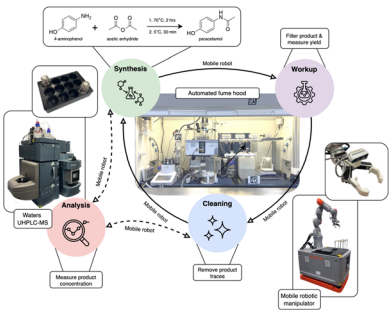
A mobile robotic process chemist

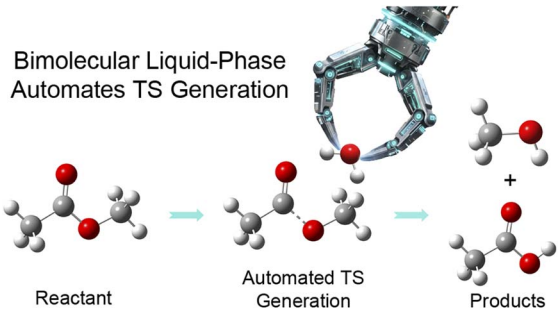
Emma J. Brass, Satheeshkumar Veeramani, Zhengxue Zhou, Hatem Fakhruldeen, J. Sebastian Manzano, Rob Clowes, Isil Akpinar, Miriam R. Ward, John W. Ward* and Andrew I. Cooper*



1372

Automated reaction transition state search for bimolecular liquid-phase reactions using internal coordinates: a test case for neutral hydrolysis

Leen Fahoum and Alon Grinberg Dana*



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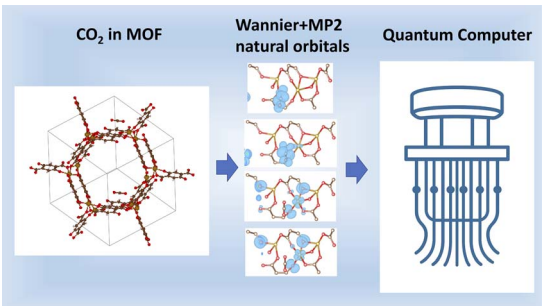
Quantum simulation of carbon capture in periodic metal–organic frameworks

Dario Rocca, Jérôme F. Gonthier, Joshua Levin, Tobias Schäfer, Andreas Grüneis, Hong Woo Lee and Byeol Kang*



1401

Chat-RFB: a flow battery chat system leveraging knowledge graphs and large language models

Hao-Tian Wang, Xuefeng Bai, Zhiling Zheng, Xin Zhang, Ruipeng Jin, Hao-Tian An, Zheng-He Xie, Xiu-Liang Lv* and Jian-Rong Li*

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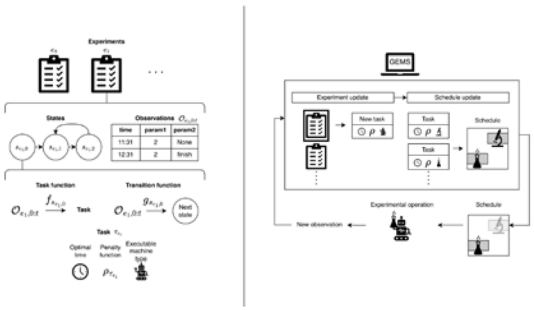

GEMS: a deterministic finite automaton framework for adaptive laboratory automation

Yuya Tahara-Arai,* Akari Kato, Koji Ochiai, Kazuya Azumi, Koichi Takahashi, Genki N. Kanda* and Haruka Ozaki*

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