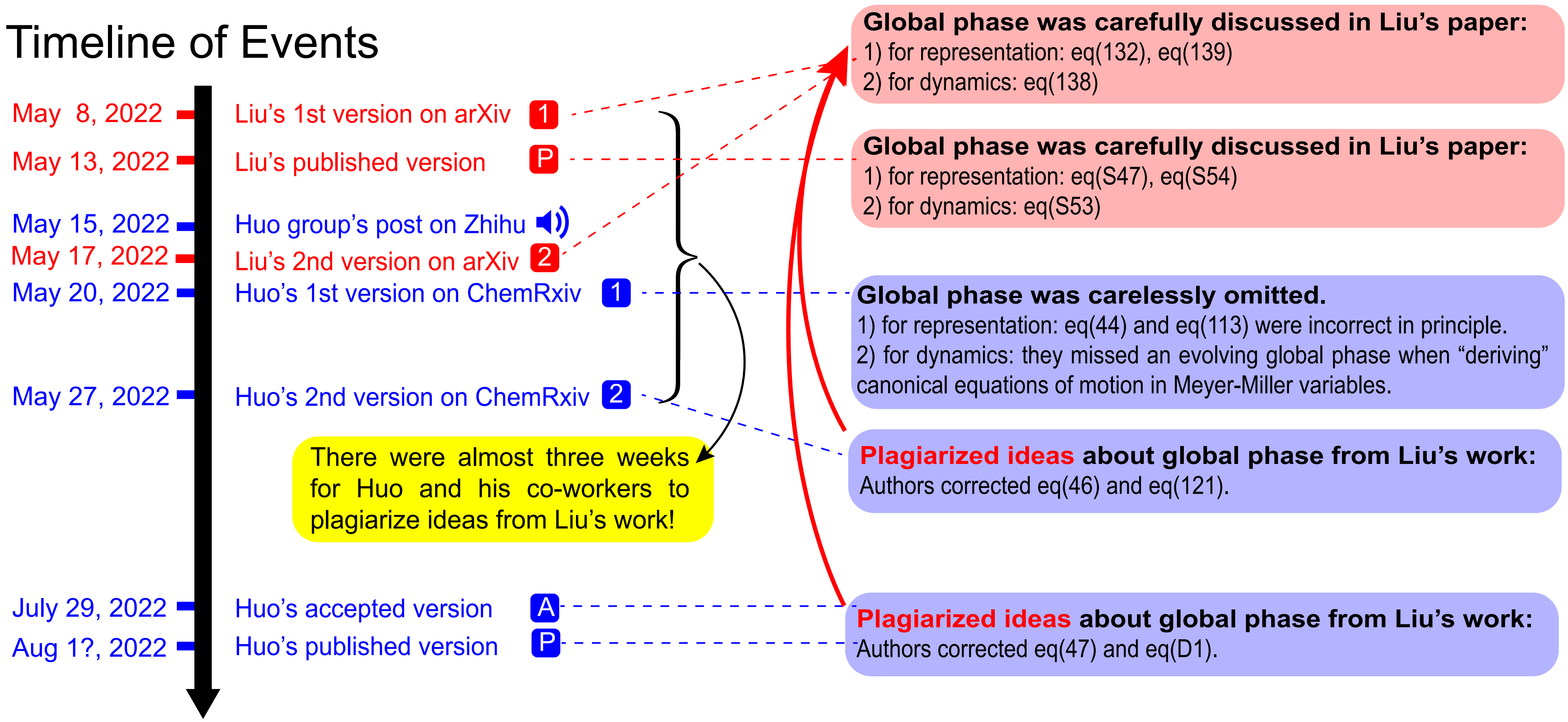

1 https://arxiv.org/abs/2205.03870v1

P https://doi.org/10.1002/wcms.1619

2 https://arxiv.org/abs/2205.03870v2

https://www.zhihu.com/people/liu-xing-yu-72-53/pins

1 https://chemrxiv.org/engage/chemrxiv/article-details/6286c9ba59f0d6831996a480

2 https://chemrxiv.org/engage/chemrxiv/article-details/6290092c1df2edd1ac59ea52

A https://aip.scitation.org/doi/10.1063/5.0094893

P https://aip.scitation.org/doi/10.1063/5.0094893

Evidence 7: PLAGIARISM

Evidence #7:

The global phase introduced around eq (46) of Version 2 (first released online to ChemRxiv on **May 27, 2022**) was totally a plagiarism from eq S54 in *Wiley Interdiscip. Rev. Comput. Mol. Sci*. e1619 (2022) [submitted on **February 5, 2022**, released on arXiv on **May 8, 2022** and officially published on **May 13, 2022**]. The global phase, linking the constraint coordinate-momentum phase space in Meyer-Miller variables and the Stratonovich phase space, had been first discussed in Appendix 3 of *Wiley Interdiscip. Rev. Comput. Mol. Sci.* e1619 (2022). In the second paragraph of page 8 of Huo's Version 1(first released online to ChemRxiv on **May 20, 2022**), they only mentioned the global phase in short, simply thinking that it would not affect *quantum dynamics*.

"

> The above transformation defined in Eq. 44 introduce an arbitrary global phase variable, such that there are $2N-1$ independent variables among $\{q_n, p_n\}$ (with one constraint subject to Eq. 53), as opposed to only $2N-2$ independent variables among $\{\theta_n, \varphi_n\}$. This is because c_n will also, in principle, contain $2N-2$ independent real variables, with one arbitrary global phase compared to the $\{\theta_n, \varphi_n\}$ angles (see Eq. 17). This global phase will not influence the quantum dynamics.

"

However, the global phase abruptly involved in some equations of Version 2-3 while completely absent in previous Version 1:

Table 1: Comparisons of Version 1 and Version 2

Version 1 (first released online to ChemRxiv on May 20, 2022)	Version 2 (first released online to ChemRxiv on May 27, 2022)
$c_n = \langle n\|\mathbf{\Omega}\rangle = \frac{1}{\sqrt{2r_s}}(q_n + ip_n), \quad (44)$	$c_n = \langle n\|\mathbf{\Omega}\rangle \boxed{\cdot\, e^{i\Phi}} = \frac{1}{\sqrt{2r_s}}(q_n + ip_n), \quad (46)$
$q_n = \sqrt{2r_s}\cdot \mathrm{Re}[\langle n\|\mathbf{\Omega}\rangle] \quad (113a)$ $p_n = \sqrt{2r_s}\cdot \mathrm{Im}[\langle n\|\mathbf{\Omega}\rangle], \quad (113b)$	$q_n = \sqrt{2r_s}\cdot \mathrm{Re}[\langle n\|\mathbf{\Omega}\rangle \boxed{\cdot\, e^{i\Phi}}], \quad (121a)$ $p_n = \sqrt{2r_s}\cdot \mathrm{Im}[\langle n\|\mathbf{\Omega}\rangle \boxed{\cdot\, e^{i\Phi}}], \quad (121b)$

Table 2: Comparisons of Version 1 and Version 3

Version 1 (first released online to ChemRxiv on May 20, 2022)	Version 3 (accepted online on July 29, 2022)

$$c_n = \langle n\vert\Omega\rangle = \frac{1}{\sqrt{2r_s}}(q_n + ip_n), \quad (44)$$	$$c_n = \langle n\vert\mathbf{\Omega}\rangle \boxed{\cdot\, e^{i\Phi}} = \frac{1}{\sqrt{2r_s}}(q_n + ip_n), \quad (47)$$
$$q_n = \sqrt{2r_s}\cdot \mathrm{Re}[\langle n\vert\mathbf{\Omega}\rangle] \quad (113a)$$ $$p_n = \sqrt{2r_s}\cdot \mathrm{Im}[\langle n\vert\mathbf{\Omega}\rangle], \quad (113b)$$	$$c_n = \langle n\vert\mathbf{\Omega}\rangle \boxed{\cdot\, e^{i\Phi}} = \frac{1}{\sqrt{2r_s}}(q_n + ip_n), \quad (D1)$$ where we introduced $q_n/\sqrt{2r_s}$ as the real part of c_n and $p_n/\sqrt{2r_s}$ as the imaginary part of c_n. This phase $e^{i\Phi}$ is a

Actually, the global phase abruptly added here had been introduced in the eq (S54) of *Wiley Interdiscip. Rev. Comput. Mol. Sci.* e1619 (2022) [submitted on **February 5, 2022**, revised on April 8, 2022, released on arXiv on **May 8, 2022** and officially published on **May 13, 2022**]:

"

$$\begin{pmatrix} x^{(n)} \\ p^{(n)} \end{pmatrix} = \sqrt{2\lambda} \boxed{\begin{pmatrix} \cos\psi & -\sin\psi \\ \sin\psi & \cos\psi \end{pmatrix}} \begin{pmatrix} \mathrm{Re}\langle n\,\vert\,\boldsymbol{\theta},\boldsymbol{\varphi}\rangle \\ \mathrm{Im}\langle n\,\vert\,\boldsymbol{\theta},\boldsymbol{\varphi}\rangle \end{pmatrix}, \quad \text{S54}$$

"

Huo *et al.* obviously plagiarized the global phase into their representation from *Wiley Interdiscip. Rev. Comput. Mol. Sci*. e1619 (2022). Moreover, a constant global phase still does **not** lead to the correct form of canonical Hamilton's equations of motion with Meyer-Miller variables (See numerical test in XXX).