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Dear Editor,

Please, find enclosed manuscript entitled "Visible light absorption of surface-modified TiO2 nanoparticles with vitamin B6: a comparative experimental and DFT study" by Tijana S. Kovač, Enis S. Džunuzović, Jasna V. Džunuzović, Bojana Milićević, Dušan N. Sredojević, Edward N. Brothers and Jovan M. Nedeljković that we wish to be considered for publication in the *Journal of the Serbian Chemical Society*.

In this manuscript, surface modification of titanium-dioxide nanoparticles with biologically active molecule pyridoxine hydrochloride (vitamin B6) was performed. Absorption onset of surface-modified TiO2 samples with vitamin B6 is red shifted by about 0.4 eV compared to unmodified ones. The mode of binding between vitamin B6 and surface Ti atoms was investigated by Fourier transform infrared spectroscopy (FTIR). From the Benesi-Hildebrand plot, the stability constant of surface complex was found to be on the order 10² M-¹. The experimental findings were supported by detailed quantum chemical calculations based on density functional theory (DFT). The excellent agreement between experimentally measured absorption and FTIR spectra of surface-modified TiO2 NPs with vitamin B6 and theoretically calculated electronic excitation and vibrational spectra of corresponding model system was found.

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We fill free to propose following experts in the field as potential reviewers:

1. Vlasta Brezova, E-mail: [vlasta.brezova@stuba.sk](mailto:vlasta.brezova@stuba.sk)

2. Vanja Kokol, E-mail: [vanja.kokol@um.si](mailto:vanja.kokol@um.si)

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We are looking forward to hear from you soon.

Sincerely yours,

Jovan M. Nedeljković